

DISCRETE MINIMISERS ARE CLOSE TO CONTINUUM MINIMISERS FOR THE INTERACTION ENERGY

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ABSTRACT. Under suitable technical conditions we show that minimisers of the discrete interaction energy for attractive-repulsive potentials converge to minimisers of the corresponding continuum energy as the number of particles goes to infinity. We prove that the discrete interaction energy Γ -converges in the narrow topology to the continuum interaction energy. As an important part of the proof we study support and regularity properties of discrete minimisers: we show that continuum minimisers belong to suitable Morrey spaces and we introduce the set of empirical Morrey measures as a natural discrete analogue containing all the discrete minimisers.

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1. INTRODUCTION

Consider a finite set of $N \geq 2$ classical particles in Euclidean space \mathbb{R}^d interacting through a pair potential $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$. If the particles are placed at points $x_1, \dots, x_N \in \mathbb{R}^d$ and have equal masses $1/N$, then their total interaction (potential)

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energy is given by

$$E_N(\mathbf{X}) := \frac{1}{2N^2} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N W(x_i - x_j), \quad (1.1)$$

where we denote $\mathbf{X} \equiv (x_1, \dots, x_N)$. We often refer to a set of positions $(x_1, \dots, x_N) \in \mathbb{R}^{Nd}$ as a *configuration*, and call E_N the *discrete interaction energy*. The gradient of W models the interaction force between two particles: $-m_x m_y \nabla W(x - y)$ is the force that a particle at x with mass m_x exerts on a particle at y with mass m_y , and accordingly we say that W is *attractive* at $x \in \mathbb{R}^d$ when $-\nabla W(x) \cdot x \leq 0$ and *repulsive* when $-\nabla W(x) \cdot x \geq 0$. The choice of masses equal to $1/N$ is of course a convenient normalisation so that the set of N particles has total mass 1. Notice that W can be assumed to be symmetric, i.e., $W(-x) = W(x)$ for all $x \in \mathbb{R}^d$, without loss of generality since symmetrising the potential does not change the energy (1.1). The sum in (1.1) is therefore halved since pairs of particles are counted twice; more importantly, self-interactions are not present in the sum, in agreement with classical physics.

A natural question regards the existence and shape of *minimisers* of this interaction energy among all possible particle configurations; that is, particle configurations whose interaction energy is the smallest possible. We also refer to these configurations as *ground states* or *discrete minimisers*, and in this paper we are mainly concerned with their shape and size as $N \rightarrow \infty$. As we rigorously show, for large N these minimisers are closely related to minimisers of the *continuum interaction energy* E defined by

$$E(\rho) = \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(x - y) d\rho(x) d\rho(y) \quad (1.2)$$

for any $\rho \in \mathcal{P}(\mathbb{R}^d)$, where $\mathcal{P}(\mathbb{R}^d)$ is the set of Borel probability measures on \mathbb{R}^d . This expression makes sense whenever W is bounded from below and measurable, in which case the value of $E(\rho)$ is a number in $\mathbb{R} \cup \{+\infty\}$. A probability measure ρ minimising (1.2) on $\mathcal{P}(\mathbb{R}^d)$ is called a *continuum minimiser*. These continuum minimisers have been the subject of several works [3, 4, 12, 22, 45] and in particular their existence, under some technical assumptions, is almost equivalent to the *instability* of the potential W [12, 45]:

Definition 1.1 (Instability). Let $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ be a measurable function which is bounded from below and such that there exists

$$W_\infty := \lim_{|x| \rightarrow \infty} W(x) \in \mathbb{R} \cup \{+\infty\}.$$

We say that W is *unstable* if there exists $\rho \in \mathcal{P}(\mathbb{R}^d)$ such that

$$E(\rho) < \frac{1}{2} W_\infty.$$

We say that W is *stable* if it is *not* unstable, i.e., if for all $\rho \in \mathcal{P}(\mathbb{R}^d)$ we have $E(\rho) \geq W_\infty/2$; we say that W is *strictly stable* if the inequality is strict.

This concept of stability is very close to the classical concept of H -stability as given for example in [43]; see Definition 5.2. For continuous potentials it was proved in [45] that they are indeed equivalent, and for potentials with a mild singularity at the origin we show in Section 5.1 that H -instability is implied by instability as given in the above

definition. We refer the reader to Section 5.1 for further details and a brief background of these concepts. In [12, 45] it was proved that under some technical assumptions (for example, under Hypotheses 1 and 2 in the next section) continuum minimisers exist if and only if there exists a probability measure ρ with $E(\rho) \leq W_\infty/2$; that is, if and only if W is unstable or there is ρ with $E(\rho) = W_\infty/2$. It is then natural to find that the same concept of instability plays a crucial role in the behaviour of discrete minimisers for large N —this constitutes the main result in our paper: *for unstable potentials, discrete minimisers approach the set of continuum minimisers as $N \rightarrow \infty$; while for strictly stable potentials, discrete minimisers grow in size without bound as $N \rightarrow \infty$.*

In order to state the main result precisely we need a few definitions. The *diameter* of a particle configuration $\mathbf{X} = (x_1, \dots, x_N) \in \mathbb{R}^{Nd}$, denoted $\text{diam } \mathbf{X}$, is just the diameter of the set $\{x_1, \dots, x_N\} \subseteq \mathbb{R}^d$ and the *empirical measure* associated to \mathbf{X} is

$$\mu_{\mathbf{X}} := \frac{1}{N} \sum_{i=1}^N \delta_{x_i},$$

with δ_x the Dirac delta measure at a point $x \in \mathbb{R}^d$. We endow the set $\mathcal{P}(\mathbb{R}^d)$ with the *narrow* topology, obtained by duality with the space of bounded continuous functions on \mathbb{R}^d , in accordance with the terminology in [2]; we discuss more the narrow topology in Section 6. We often identify $\mathbf{X} \in \mathbb{R}^{Nd}$ with its empirical measure $\mu_{\mathbf{X}}$, and accordingly we use on \mathbf{X} concepts that really apply to $\mu_{\mathbf{X}}$. For example, we say that a sequence $(\mathbf{X}_N)_{N \geq 2}$, with $\mathbf{X}_N \in \mathbb{R}^{Nd}$ for all $N \geq 2$, converges to ρ (narrowly) if $\mu_{\mathbf{X}_N}$ converges to ρ in the narrow topology. Postponing the precise hypotheses to Section 2, the following is our main result:

Theorem 1.2 (Main result). *Assume that W satisfies Hypotheses 1, 2 and 3 in Section 2. For any $N \geq 2$ the discrete energy E_N has a minimiser on \mathbb{R}^{Nd} , and for any sequence $(\mathbf{X}_N)_{N \geq 2}$ of such minimisers the following statements hold:*

- (1) *If W is unstable, then the diameter of \mathbf{X}_N is uniformly bounded for all N and $(\mathbf{X}_N)_{N \geq 2}$ has a subsequence which converges in the narrow sense, up to translations, to a minimiser of the continuum energy E as $N \rightarrow \infty$.*
- (2) *If W is strictly stable, then the diameter of \mathbf{X}_N tends to ∞ as $N \rightarrow \infty$.*

The case in which $\inf_{\rho \in \mathcal{P}(\mathbb{R}^d)} E(\rho) = \min_{\rho \in \mathcal{P}(\mathbb{R}^d)} E(\rho) = (1/2) \lim_{|x| \rightarrow \infty} W(x)$, that is, the case in which W is stable but not strictly stable, is not included in our main result. Indeed this is a critical case for which our approach is not conclusive; discrete minimisers may still exist for every N but we cannot get a uniform bound on their diameter, which prevents us from proving convergence to a continuum minimiser. The precise hypotheses on W are given in Section 2 but we already point out that the *power-law* potentials

$$W(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b} \quad \text{with} \quad \begin{cases} 0 < b < a & \text{when } d \in \{1, 2\}, \\ 2 - d < b < a, \quad b \neq 0, & \text{when } d \geq 3, \end{cases} \quad (1.3)$$

satisfy all assumptions in the main theorem and are unstable (and thus their associated discrete minimisers behave as Theorem 1.2(1)). The *Morse potentials*

$$W(x) = C_r \exp(-|x|/\ell_r) - C_a \exp(-|x|/\ell_a), \quad (1.4)$$

for some positive constants C_r, ℓ_r, C_a and ℓ_a , also satisfy all assumptions and are unstable if $\ell_r < \ell_a$ and $C_r/C_a < (\ell_a/\ell_r)^d$; see [12, Proposition 3.2].

Theorem 1.2 gives a natural link between the discrete energy (1.1) and the continuum one (1.2). In the same way as [12, 45] showed that strict stability is the property of the potential that determines existence or not of continuum minimisers, Theorem 1.2 shows that it also determines the existence or not of a limit of the family of discrete minimisers as $N \rightarrow \infty$. In fact our proof follows “discrete versions” of arguments in [12]. Regularity results for continuum minimisers in [3] are also crucial and our proof contains discrete analogues of these. Let us now give some background motivation for the problem we are considering and then let us sketch the strategy of our proof.

Previous results and motivation. Discrete minimisers represent the natural minimal energy configurations of N particles under the given potential in the absence of any external forces and without thermal fluctuations (in other words, these are classical ground states at temperature 0). Understanding the shape of these ground states (and those of related energy functionals) when the number N of particles is very large is of obvious interest in statistical mechanics [42, 44, 46], with direct implications in materials science [32, 38, 39, 41]. For physically relevant potentials such as the Lennard-Jones potential $W(x) = |x|^{-12} - |x|^{-6}$ the conjectured behaviour is that *crystallisation* takes place as $N \rightarrow \infty$. That is: minimisers have particles placed almost at the vertices of a regular triangular lattice, approaching the lattice as N increases. This has been rigorously proved for certain potentials similar to Lennard-Jones in dimensions 1 and 2 [31, 46] and for some other very specific potentials [38, 39], but is in general an unsolved problem; for results in this direction, see also [42] for some interaction energies with an external confining potential and [44] for systems with Coulomb interactions and their links to other mathematical problems. Even if showing a crystallisation property is remarkably hard, one can make a weaker observation: for certain potentials, including Lennard-Jones, the *diameter* of ground states seems to increase without bound as $N \rightarrow \infty$, while for others the diameter seems to tend to a fixed value. This is part of the content of Theorem 1.2, whose main restriction in this setting is that it essentially requires the potential W to be less singular than $|x|^{2-d}$ at $x = 0$ (such as for example (1.3)). When the singularity is stronger, between $|x|^{-d}$ and $|x|^{2-d}$, we expect our main result still to be true, although we are unable to show it since potentials in this case do not satisfy Hypothesis 3. Hence our statement does not say anything about the Lennard-Jones case, but does show that minimisers grow in diameter without bound for a range of stable potentials with a possible singularity at $x = 0$.

In addition to their relevance in statistical mechanics, an important more recent motivation for our results comes from the field of collective behaviour, where shapes of self-organised structures in some individual-based models exhibit very interesting phenomena and are closely related to those of discrete minimisers [1, 6, 19, 25, 37, 48]; see the survey on emergent behaviour [36] and the references therein. In this context, models aim at capturing the behaviour of a large number of individuals, with applications to fish, cattle, birds, ants, and crowds of people. In very simplified models, interaction through a potential reflects a tendency of individuals to avoid close contact while keeping a tendency to stay close to the group. The study of these models has

led to different questions regarding the minimisers of (1.1), mainly since the potentials involved are not determined by physics but by phenomenological considerations in each particular model. This has sparked interest in the shape of minimisers for potentials which are very different from those found in physics, including potentials with a mild or no singularity at 0 or which tend to infinity at large distances. The paper [25] is the first example we know of where the link was made between the stability properties of the potential and the size of stationary states for a potential interaction. In it, a particular time-dependent interaction model was considered with the Morse potential (1.4) and its asymptotic states were numerically studied. It was observed that their size increases with N for stable potentials while it does not for unstable ones. This is precisely the behaviour which Theorem 1.2 aims at justifying rigorously.

Minimisers of the continuum energy (1.2) are also of interest in collective behaviour models [14, 28, 29], in the theory of nonlocal partial differential equations [9–11], and again in connection to statistical mechanics [5]. They display interesting effects such as a link between the repulsive singularity of the potential and smoothness of minimisers [3, 9, 26, 27]; they are connected to solutions to obstacle problems in certain cases [17, 20]; and for specific potentials W they are also linked to the theory of random matrices [21]. These continuum minimisers are often studied by numerically solving an N -particle approximation, with the assumption that stationary states for large N are good approximations to the continuum ones. As far as we know, our present results are the first where a justification of this is given. Of course, in order to make the results practical for numerical simulation it would be very useful to estimate the rate of convergence to continuum minimisers as $N \rightarrow \infty$ in Theorem 1.2; this seems a worthwhile but difficult question, since even the uniqueness of minimisers is unclear (except for specific potentials W [11, 28]).

Let us mention as well that the connection between the discrete and continuum energies is a hard question in mean-field limit results for dynamical problems [13, 15, 16, 18, 34], especially for potentials which have a singularity at $x = 0$. Roughly speaking, the main difficulty is to show that the unbounded forces between particles resulting from the singularity are in fact negligible for large N if one only cares about the overall particle density. Unsurprisingly, our proof is much more delicate for singular potentials and yields more interesting estimates at the discrete level in that case.

Strategy of proof. Our general strategy is based on drawing a parallel discrete version of several results which have been recently obtained for continuum minimisers. A first one is the *regularity* of continuum minimisers, studied in [3, 9, 17]. We describe this informally now and we refer the reader to Section 3 for full details. If the potential W behaves like $-|x|^b/b$ close to $x = 0$ for some $2 - d < b < 2$, then it was proved in [3] that the dimension of the support of continuum minimisers is at least $2 - b$. In fact, a stronger regularity result is a direct consequence of the arguments in [3], though it was not explicitly remarked there: it holds that $|x|^{b-2} * \rho$ is a bounded function for any minimiser ρ and hence one obtains (see Section 3) that ρ is in the Morrey space of measures which satisfy

$$\rho(B_r) \leq Cr^{2-b}$$

for any ball B_r of radius $r > 0$, and some $C > 0$ independent of the ball B_r . Now, an analogue of this regularity is needed for discrete minimisers $\mathbf{X} = (x_1, \dots, x_N) \in \mathbb{R}^{Nd}$, with the difficulty that the empirical measure

$$\mu_{\mathbf{X}} := \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$$

cannot satisfy the same bound, being a sum of Dirac delta functions. Instead of this, we prove the following variation: the total mass of particles inside a ball of radius r *centred at one of the particles* is less than a constant times r^{2-b} if one does not count the particle at the center. In other words, there exists a universal constant $C > 0$ depending only on W such that

$$\mu_{\mathbf{X}}(B_r(x_i)) \leq Cr^{2-b} + \frac{1}{N} \quad \text{for } i \in \{1, \dots, N\} \quad (1.5)$$

for any discrete minimiser $\mathbf{X} = (x_1, \dots, x_N) \in \mathbb{R}^{Nd}$ (always under the assumption that $W(x) \sim -|x|^b/b$ for $x \sim 0$). This motivates an interesting definition of “empirical Morrey measures” which serves as a discrete version of the Morrey spaces; see Sections 3 and 4 for details.

Another important basic property of continuum minimisers is that they satisfy the following conditions, as proved in [3] (and informally noticed in [5] without a rigorous proof): if a probability measure ρ minimises (1.2) then

$$\begin{cases} W * \rho(x) = 2E(\rho) & \text{for } \rho\text{-almost every } x \in \mathbb{R}^d, \\ W * \rho(x) \geq 2E(\rho) & \text{for almost every } x \in \mathbb{R}^d. \end{cases} \quad (1.6)$$

The quantity $W * \rho(x)$ represents the potential created by the mass distribution ρ at the point $x \in \mathbb{R}^d$; the above statement says in particular that it is almost everywhere constant in the support of ρ . We refer to the condition in the first line as the *Euler–Lagrange* equation. The quantity corresponding to $W * \rho(x)$ in the discrete case, for a particle distribution $\mathbf{X} \in \mathbb{R}^{Nd}$, is

$$P_i(\mathbf{X}) := \frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^N W(x_i - x_j) \quad \text{for all } i \in \{1, \dots, N\},$$

which is the potential at position x_i created by all particles but that at x_i . Interestingly, for a discrete minimiser this does *not* seem to be constant at all sites i , but we show a bound on its variation across sites which decays asymptotically as $N \rightarrow \infty$: there exist $A > 0$ and $0 < k \leq 1$ such that

$$|P_i(\mathbf{X}) - P_j(\mathbf{X})| \leq AN^{-k} \quad \text{for all } i, j \in \{1, \dots, N\} \quad (1.7)$$

for any discrete minimiser $\mathbf{X} \in \mathbb{R}^{Nd}$. The constants A and k are independent of N (and are constructive) and thus this shows that for large N the potential at two different particles cannot differ by a large amount.

Finally, continuum minimisers are known to be compactly supported if W is increasing at long range, with a constructive bound as proved in [12]. Analogously, in Section 4.4 we give a uniform bound on the diameter of discrete minimisers, which can be

understood as a discrete version of the argument in [12], using the approximate Euler–Lagrange property (1.7) and the “discrete Morrey regularity” (1.5). We point out that the latter is needed only for potentials which are unbounded at $x = 0$, which are the main difficulty in our result.

We also phrase some of our results using the terminology of Γ -convergence in Section 6. Our proof of convergence of minimisers contains the fact that the discrete energy (1.1) Γ -converges to the continuum energy (1.2) in the narrow topology, which depends on the singularity of the potential W . We remark that there is a previous related result in [23], where the Γ -convergence of the *regularised* continuum energy (associated to a mollified potential W_ϵ) to the energy (1.2) (associated to W) was studied as the regularisation parameter ϵ tends to 0. Hence this latter result is concerned with convergence of the continuum energy (1.2) for different potentials, while in the present paper we study the convergence of the discrete energy (1.1) as $N \rightarrow \infty$ for a fixed potential W .

The structure of the paper is as follows. In Section 2 we gather some necessary definitions and state precisely our hypotheses. Section 3 contains some simple observations on the regularity of continuum minimisers, directly deduced from [3]. Section 4 gathers several properties of discrete minimisers, including existence, “discrete regularity” (a discrete version of the continuum one) and an approximate Euler–Lagrange property. Finally, in Section 5 the proof of our main result is completed, showing that discrete minimisers approach the set of continuum ones as the number of particles goes to infinity. In Section 6 we prove a technical result that is needed in earlier proofs: the discrete energy Γ -converges to the continuum one; essentially, we show that one may approximate a probability measure ρ by a discrete distribution in such a way that the interaction energy is also approximated if ρ has a suitable Morrey regularity.

2. PRELIMINARIES AND HYPOTHESES

In order to state the full assumptions in our results we need to introduce a couple of definitions. The first is the concept of β -repulsivity, taken from [3]. For any $R \geq 0$ and $z \in \mathbb{R}^d$ we denote by $B_R(z)$ the open ball of radius R and centre z ; in the case $z = 0$ we simply write B_R . Analogously, we write $\overline{B}_R(z)$, or \overline{B}_R , for the closed ball. The integral \int_A denotes the averaged integral over a region A , that is, \int_A divided by the Lebesgue measure of A .

Definition 2.1 (Approximate and generalised Laplacians). Let $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ be a locally integrable function. The *approximate Laplacian* of W is defined, for all $\varepsilon > 0$, by

$$\Delta^\varepsilon W(x) = \frac{2(d+2)}{\varepsilon^2} \left(\int_{B_\varepsilon} W(x+y) dy - W(x) \right) \quad \text{for all } x \in \mathbb{R}^d,$$

and the *generalised Laplacian* of W is defined by

$$\Delta^0 W(x) = \liminf_{\varepsilon \rightarrow 0} \Delta^\varepsilon W(x) \quad \text{for all } x \in \mathbb{R}^d.$$

Note that $\Delta^\varepsilon W$ makes sense as a number in $\mathbb{R} \cup \{+\infty\}$, and $\Delta^0 W$ may be a number in $\mathbb{R} \cup \{-\infty, +\infty\}$. Also, if the classical Laplacian of W exists at some $x \in \mathbb{R}^d$, then $\Delta W(x) = \Delta^0 W(x)$.

Definition 2.2 (β -repulsivity). Let $\beta > 0$ and $W : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$. We say that W is β -repulsive at the origin if it is locally integrable and there exist $\delta > 0$ and $C > 0$ such that

$$-\Delta^0 W(x) \begin{cases} \geq C|x|^{-\beta} & \text{for all } x \in \mathbb{R}^d \text{ with } 0 < |x| < \delta, \\ = +\infty & \text{for } x = 0. \end{cases} \quad (2.1)$$

Notice that the notion of β -repulsivity is sensitive to the value of W at $x = 0$, so it does not hold if we arbitrarily set $W(0) := W_0 \in \mathbb{R}$ when W is lower semicontinuous (the second line of (2.1) would not be satisfied). Typically, potentials with a singularity equal to or stronger than the Newtonian are generally *not* β -repulsive for any $\beta > 0$. Indeed, if $W(x) := -|x|^b/b$ for $b \neq 2-d$ (with the understanding that $|x|^0/0 = \log|x|$), one can easily check that $\Delta W(x) = (2-b-d)|x|^{b-2}$ for all $x \neq 0$, which leads to a violation of the first line of (2.1) if $b < 2-d$. If $b = 2-d$, then ΔW is a multiple of the Dirac measure at the origin and (2.1) again cannot be satisfied; the Newtonian potential is therefore not β -repulsive, for any $\beta > 0$. On the opposite, if $2-d < b < 2$, that is, if W has a milder singularity than the Newtonian potential, then it is β -repulsive with $\beta = 2-b$.

Our first assumption on W is the most basic, ensuring that the interaction energies we use are well defined and have suitable lower semicontinuity properties:

Hypothesis 1. $W : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is measurable, lower semicontinuous, bounded from below by a finite constant $W_{\min} \in \mathbb{R}$, and locally integrable.

In order to prove existence of discrete minimisers we need to add the following assumption, whose main point is to ensure that W is attractive at long distances:

Hypothesis 2. There exists $\lim_{|x| \rightarrow \infty} W(x) =: W_\infty \in \mathbb{R} \cup \{+\infty\}$, W is symmetric, and there is $R_W > 0$ such that W is radially strictly increasing on $\mathbb{R}^d \setminus B_{R_W}$.

As mentioned in the introduction, the condition on the symmetry of W implies no loss of generality since nonsymmetric potentials can be symmetrised without changing the value of the interaction energy. Finally, in order to show a uniform bound on the support of discrete minimisers we need to assume a specific behaviour of the potential at the origin:

Hypothesis 3. One of the two following properties holds:

Hypothesis 3a. W is bounded from above and upper semicontinuous.

Hypothesis 3b. W is β -repulsive for some $2 < \beta < d$, it belongs to $\mathcal{C}^1(\mathbb{R}^d \setminus \{0\})$, and for some $C_W > 0$ we have

$$\begin{aligned} \Delta^0 W(x) &\leq C_W && \text{for all } x \in \mathbb{R}^d, \\ W(x) &\leq C_W |x|^{2-\beta} && \text{for all } |x| \leq 1, \\ |\nabla W(x)| &\leq C_W |x|^{1-\beta} && \text{for all } |x| \leq 1. \end{aligned}$$

Notice that Hypothesis 3a and the lower semicontinuity and boundedness from below of Hypothesis 1 imply that $W \in \mathcal{C}(\mathbb{R}^d)$. Hypothesis 3a tells us that $W(0)$ is bounded, whereas Hypothesis 3b includes unbounded potentials with a specific repulsive behaviour at the origin. The radius 1 in the bounds of W and $|\nabla W|$ is not

fundamental and all proofs work with minor modifications if these bounds hold for $|x| < r_0$ for a given positive r_0 . Since we must require that W satisfies Hypotheses 1–3, we obtain our results for singularities up to, and not including, that of the Newtonian potential $|x|^{2-d}/(d-2)$ (or $-\log|x|$ when $d=2$), with the main restriction coming from Hypothesis 3b.

Typically, the potentials of interest are attractive at long ranges and repulsive at short ones, and are smooth away from 0 with a possible singularity at the origin. As already mentioned, a class of potentials satisfying Hypotheses 1–3 consists of the power-law combinations (1.3), where we set $W(0) = +\infty$ if $b < 0$. Notice that Hypothesis 3a covers the cases with $b \geq 0$, while Hypothesis 3b covers the cases with $b < 0$. When $d \in \{1, 2\}$ all power-law potentials of the type (1.3) fall in the case of Hypothesis 3a due to the condition $0 < b$; in dimensions 1 and 2 the functions $|x|^b$ are not β -repulsive (for any β) if $b \leq 0$.

Let us finally make a note in this section of the terminology used. As it is clear from the introduction, we refer in this paper to *global* minimisers (of the continuum or discrete energy) simply as minimisers. This is because we are not concerned with local minimisers, except on some limited occasions where we clearly mention it as well as the underlying topology in the continuum case. Also, we say that $\rho \in A \subset \mathcal{P}(\mathbb{R}^d)$ is a minimiser of the continuum energy *on* the set A if it minimises the energy among all elements of A ; this holds in the discrete setting too.

3. REGULARITY OF CONTINUUM MINIMISERS

We make a short observation on the regularity of continuum minimisers which is essentially contained in the results of [3], but is not mentioned there explicitly. Later, in Section 4.2, we carry out a discrete version of these arguments. Our main result on continuum minimisers states that they are bounded in a specific Morrey space of measures for β -repulsive potentials. We always denote by $\mathcal{M}(\mathbb{R}^d)$ the space of finite (signed) Borel measures on \mathbb{R}^d .

Definition 3.1 (Morrey spaces). Let $p \in [1, \infty]$ and $\rho \in \mathcal{M}(\mathbb{R}^d)$. We say that ρ belongs to the *p-Morrey space* $\mathcal{M}_p(\mathbb{R}^d)$ if there exists a constant $M > 0$ such that, for all $r > 0$ and $x \in \mathbb{R}^d$,

$$|\rho|(B_r(x)) \leq Mr^{d/q},$$

where q is the Hölder dual of p and $|\rho|(A)$ is the total variation of ρ in a Borel set $A \subset \mathbb{R}^d$. For any $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ we define its *p-Morrey norm* by

$$\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} = \sup \{ r^{-d/q} |\rho|(B_r(x)) \mid (r, x) \in (0, \infty) \times \mathbb{R}^d \}.$$

Observe that for $p = 1$ we have $q = +\infty$ and the above definition just states that ρ is finite, so $\mathcal{M}_1(\mathbb{R}^d)$ is just $\mathcal{M}(\mathbb{R}^d)$ with the total variation norm. Similarly, for $p = \infty$ we have $q = 1$ and $\mathcal{M}_\infty(\mathbb{R}^d)$ can be identified with $L^\infty(\mathbb{R}^d)$.

Theorem 3.2. *Assume that W satisfies Hypothesis 1, it is β -repulsive for some $0 < \beta < d$ and $\Delta^0 W \leq C_W$ for some $C_W > 0$. If $\rho \in \mathcal{P}(\mathbb{R}^d)$ is a minimiser of the continuum interaction energy E , then $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ with $p = d/(d - \beta)$ and $\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} \leq 2^\beta C'$ for some $C' > 0$ only depending on W .*

Note that if $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ then the Hausdorff dimension of the support of ρ is bounded from below by d/q by Frostman's lemma [40]; Theorem 3.2 thus tells us that the dimension of the support of a continuum minimiser is at least β . This dimensionality property is one of the main results in [3] and our observation is that almost the same argument used in [3] actually reaches the stronger conclusion that $\rho \in \mathcal{M}_p(\mathbb{R}^d)$. Theorem 3.2 is directly deduced from the next three lemmas. The first one can be readily found in [3, Corollary 1]. The second one states that a minimiser can be convolved with $|\cdot|^{-\beta}$ to give a bounded function, and is proved by following and adapting the proof of [3, Proposition 3]. The third one comes from potential theory and states that a probability measure ρ whose convolution with $|\cdot|^{-\beta}$ is bounded is p -Morrey regular for $p = d/(d - \beta)$; it can be found for example in [40, Section 8]).

Lemma 3.3 (see [3, Corollary 1]). *Let W satisfy Hypothesis 1 and suppose that $\Delta^0 W \leq C_W$ for some $C_W > 0$. If ρ is a minimiser of E , then $\Delta^0 W * \rho(x) \geq 0$ for all $x \in \text{supp } \rho$.*

Lemma 3.4. *Let W be as in Theorem 3.2 and let $\rho \in \mathcal{P}(\mathbb{R}^d)$ be a minimiser of the continuum energy. There exists a constant $C' > 0$ (depending only on W) such that*

$$\int_{\mathbb{R}^d} |x - y|^{-\beta} d\rho(y) \leq C' \quad \text{for all } x \in \text{supp } \rho.$$

Proof. Choose $x_0 \in \text{supp } \rho$ and write $\rho = \rho_0 + \rho_1$, with ρ_0 and ρ_1 two nonnegative measures such that $\text{supp } \rho_0 \subset B_\delta(x_0)$ and $\text{supp } \rho_1 \subset \mathbb{R}^d \setminus B_\delta(x_0)$, where δ is as in Definition 2.2, and such that neither ρ_0 nor ρ_1 are zero measures. Now compute

$$\begin{aligned} C \int_{\mathbb{R}^d} |x_0 - y|^{-\beta} d\rho_0(y) &\leq - \int_{\mathbb{R}^d} \Delta^0 W(x_0 - y) d\rho_0(y) \\ &= - \int_{\mathbb{R}^d} \Delta^0 W(x_0 - y) d\rho(y) + \int_{\mathbb{R}^d} \Delta^0 W(x_0 - y) d\rho_1(y) \\ &= -\Delta^0 W * \rho(x_0) + \int_{\mathbb{R}^d} \Delta^0 W(x_0 - y) d\rho_1(y) \\ &\leq \int_{\mathbb{R}^d} \Delta^0 W(x_0 - y) d\rho_1(y) \leq C_W, \end{aligned}$$

using the β -repulsivity of W with C as in Definition 2.2, the fact that $\Delta^0 W * \rho(x) \geq 0$ for all $x \in \text{supp } \rho$ by Lemma 3.3, $\Delta^0 W \leq C_W$, and $\rho_1(\mathbb{R}^d) \leq 1$. Therefore

$$\begin{aligned} \int_{\mathbb{R}^d} |x_0 - y|^{-\beta} d\rho(y) &\leq \frac{C_W}{C} + \int_{\mathbb{R}^d} |x_0 - y|^{-\beta} d\rho_1(y) \leq \frac{C_W}{C} + \int_{\mathbb{R}^d \setminus B_\delta(x_0)} |x_0 - y|^{-\beta} d\rho_1(y) \\ &\leq \frac{C_W}{C} + \delta^{-\beta} =: C', \end{aligned}$$

using that $\beta > 0$ and $\rho_1(\mathbb{R}^d \setminus B_\delta(x_0)) \leq 1$. Notice that the constant C' is independent of x_0 . Thus, since the choice of $x_0 \in \text{supp } \rho$ is arbitrary, we get the desired result. \blacksquare

Lemma 3.5. *Let $0 < \beta < d$ and $\rho \in \mathcal{P}(\mathbb{R}^d)$. Suppose that there is a constant $C' > 0$ with*

$$\int_{\mathbb{R}^d} |x - y|^{-\beta} d\rho(y) \leq C' \quad \text{for all } x \in \text{supp } \rho.$$

Then $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ with $p = d/(d - \beta)$ and $\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} \leq 2^\beta C'$.

Proof. Let $r > 0$. Then, for all $x \in \text{supp } \rho$,

$$r^{-\beta} \rho(B_r(x)) \leq \int_{B_r(x)} |x - y|^{-\beta} d\rho(y) \leq \int_{\mathbb{R}^d} |x - y|^{-\beta} d\rho(y) \leq C',$$

since $\beta > 0$. Now suppose that $x \notin \text{supp } \rho$. Then, either $\rho(B_r(x)) = 0$ or $\rho(B_r(x)) > 0$. In the former case, we get $r^{-\beta} \rho(B_r(x)) \leq C'$ trivially. In the latter, we know that there exists $z \in \text{supp } \rho \cap B_r(x)$ with $\rho(B_r(x)) \leq \rho(B_{2r}(z))$. Hence, by the inequality above applied to z and $2r$,

$$r^{-\beta} \rho(B_r(x)) \leq r^{-\beta} \rho(B_{2r}(z)) \leq 2^\beta (2r)^{-\beta} \rho(B_{2r}(z)) \leq 2^\beta C'.$$

Therefore, writing $M := 2^\beta C'$, we have the result:

$$\rho(B_r(x)) \leq M r^\beta = M r^{d(1-1/p)} \quad \text{for all } x \in \mathbb{R}^d. \quad \blacksquare$$

The previous three lemmas easily imply Theorem 3.2. For later use we give the following additional lemma, which is almost a converse of Lemma 3.5. It involves a relatively well-known argument, and can be found for example in [30, Lemma 2.1]:

Lemma 3.6. *Let $p > 1$, $q = p/(p-1)$ and $0 < \beta < d/q$. For all $r > 0$, there exists $C_r > 0$ (depending only on β , r , q and d) such that $C_r \rightarrow 0$ as $r \rightarrow 0$ and, for all $\rho \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$,*

$$\int_{B_r(x)} |x - y|^{-\beta} d\rho(y) \leq C_r \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} \quad \text{for all } x \in \mathbb{R}^d.$$

Proof. Let $r > 0$ and $x \in \mathbb{R}^d$, and write $D_i(x) := \{y \in \mathbb{R}^d \mid 2^{-i-1}r \leq |x - y| \leq 2^{-i}r\}$ for all $i \in \{0, 1, 2, \dots\}$. Compute

$$\begin{aligned} \int_{B_r(x)} |x - y|^{-\beta} d\rho(y) &= \sum_{i=0}^{\infty} \int_{D_i(x)} |x - y|^{-\beta} d\rho(y) \leq \sum_{i=0}^{\infty} 2^{(i+1)\beta} r^{-\beta} \int_{D_i(x)} d\rho(y) \\ &\leq \sum_{i=0}^{\infty} 2^{(i+1)\beta} r^{-\beta} \int_{\{y \in \mathbb{R}^d \mid 0 \leq |x-y| \leq 2^{-i}r\}} d\rho(y) \\ &= \sum_{i=0}^{\infty} 2^{(i+1)\beta} r^{-\beta} \rho(B_{2^{-i}r}(x)) \\ &\leq \sum_{i=0}^{\infty} 2^{(i+1)\beta} r^{-\beta} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} 2^{-id/q} r^{d/q} \\ &= 2^\beta r^{d/q-\beta} \sum_{i=0}^{\infty} 2^{i(\beta-d/q)} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)}. \end{aligned}$$

Since $\beta < d/q$ we know $\sum_{i=0}^{\infty} 2^{i(\beta-d/q)}$ is finite. Setting $C_r := 2^\beta r^{d/q-\beta} \sum_{i=0}^{\infty} 2^{i(\beta-d/q)}$ therefore gives the result. \blacksquare

Let us remark that Theorem 3.2 actually holds when $\rho \in \mathcal{P}(\mathbb{R}^d)$ has finite energy and it is a local minimiser of the continuum energy with respect to the Wasserstein distance of any finite or infinite order, since Lemma 3.3 stays true in this case; see [3, Corollary 1], and [2, 47] for an account on transport distances. Wasserstein local minimisers of

the continuum energy are therefore Morrey regular under the assumptions on W of Theorem 3.2.

4. PROPERTIES OF DISCRETE MINIMISERS

4.1. **Existence.** Let us prove the first part of the main result, Theorem 1.2, regarding the existence of minimisers of the discrete interaction energy:

Theorem 4.1. *Assume Hypotheses 1 and 2. For any $N \geq 2$ the discrete energy E_N has a minimiser on \mathbb{R}^{Nd} . Furthermore, the diameter of any such minimiser is less than $K_N := 2\sqrt{d}(N-1)R_W$ (which only depends on N and W).*

Theorem 4.1 is proved by considering minimisers in $(\overline{B}_R)^N$ for some $R \geq 0$, and by showing a uniform bound on their diameter, independently of R . This is stated in the following lemma:

Lemma 4.2. *Suppose that W satisfies Hypotheses 1 and 2, and let $R \geq 0$. There exists a minimiser of E_N on $(\overline{B}_R)^N$. If \mathbf{X} is any such minimiser, then*

$$\text{diam } \mathbf{X} \leq 2\sqrt{d}(N-1)R_W =: K_N.$$

Observe that our control of the support of the minimiser given by Lemma 4.2 depends on N . This is an easy estimate which holds under weak conditions on W ; later, in Theorem 4.12, we show that in fact, when W is unstable, the size of the support of N -particle minimisers stays uniformly bounded in N , and that constitutes one of the central arguments in this paper.

Proof of Lemma 4.2. The fact that a minimiser exists is straightforward by compactness of $(\overline{B}_R)^N$ and lower semicontinuity of E_N (since W is lower semicontinuous). Let then \mathbf{X} be a minimiser of E_N on $(\overline{B}_R)^N$.

Denote by $\pi_k: \mathbb{R}^d \rightarrow \mathbb{R}$ the projection on the k th axis. We want to prove the following claim. In each coordinate there cannot be “gaps” greater than $2R_W$ among any particles of \mathbf{X} : if $k \in \{1, \dots, d\}$ and $a_k \in \mathbb{R}$ is so that $x_i \notin \pi_k^{-1}([a_k - R_W, a_k + R_W])$ for all $i \in \{1, \dots, N\}$, then either $x_i \notin \pi_k^{-1}((-\infty, a_k - R_W])$ for all $i \in \{1, \dots, N\}$ or $x_i \notin \pi_k^{-1}([a_k + R_W, \infty))$ for all $i \in \{1, \dots, N\}$. Without loss of generality we prove the claim for $k = 1$. We proceed by contradiction: assume that there is $a_1 \in \mathbb{R}$ such that $I_L := \{i \in \{1, \dots, N\} \mid x_i \in \pi_1^{-1}((-\infty, a_1 - R_W])\} \neq \emptyset$, $I_R := \{i \in \{1, \dots, N\} \mid x_i \in \pi_1^{-1}([a_1 + R_W, \infty))\} \neq \emptyset$ and $\{1, \dots, N\} \setminus (I_L \cup I_R) = \emptyset$. By renaming the particles we may assume that $I_L = \{1, \dots, N_L\}$ and $I_R = \{N_L + 1, \dots, N\}$ for some $1 \leq N_L < N$. Let $0 < \varepsilon_1 \leq R_W$ and $\varepsilon = (\varepsilon_1, 0, \dots, 0) \in \mathbb{R}^d$, and define the “left-shifted” particles

$$\mathbf{X}' = (x'_1, \dots, x'_N) := (x_1, \dots, x_{N_L}, x_{N_L+1} - \varepsilon, \dots, x_N - \varepsilon) \in (\overline{B}_R)^N.$$

Let us compute the discrete energy of \mathbf{X}' .

$$\begin{aligned} N^2 E_N(\mathbf{X}') &= \frac{1}{2} \sum_{i \in I_L} \sum_{\substack{j \in I_L \\ j \neq i}} W(x'_i - x'_j) + \frac{1}{2} \sum_{i \in I_R} \sum_{\substack{j \in I_R \\ j \neq i}} W(x'_i - x'_j) + \sum_{i \in I_L} \sum_{j \in I_R} W(x'_i - x'_j) \\ &= \frac{1}{2} \sum_{i \in I_L} \sum_{\substack{j \in I_L \\ j \neq i}} W(x_i - x_j) + \frac{1}{2} \sum_{i \in I_R} \sum_{\substack{j \in I_R \\ j \neq i}} W(x_i - \varepsilon - (x_j - \varepsilon)) \end{aligned}$$

$$+ \sum_{i \in I_L} \sum_{j \in I_R} W(x_i - x_j + \varepsilon).$$

Let $x_{i,1} := \pi_1(x_i)$ for any $i \in \{1, \dots, N\}$. Since clearly $x_{i,1} - x_{j,1} + \varepsilon_1 \leq -2R_W + \varepsilon_1 \leq -R_W$ for all $(i, j) \in I_L \times I_R$, Hypothesis 2 gives

$$\begin{aligned} N^2 E_N(\mathbf{X}') &< \frac{1}{2} \sum_{i \in I_L} \sum_{\substack{j \in I_L \\ j \neq i}} W(x_i - x_j) + \frac{1}{2} \sum_{i \in I_R} \sum_{\substack{j \in I_R \\ j \neq i}} W(x_i - x_j) + \sum_{i \in I_L} \sum_{j \in I_R} W(x_i - x_j) \\ &= N^2 E_N(\mathbf{X}), \end{aligned}$$

which is a contradiction of \mathbf{X} being a minimiser on $(\overline{B}_R)^N$, which shows the claim.

To complete the proof of the lemma note that the above claim implies that the diameter of the k th projection of the set $\{x_1, \dots, x_N\}$ is less than $2(N-1)R_W$. Since this is true of all projections, we deduce that $\text{diam}\{x_1, \dots, x_N\} \leq 2\sqrt{d}(N-1)R_W$, which ends the proof. \blacksquare

We can now prove Theorem 4.1.

Proof of Theorem 4.1. By Lemma 4.2 we know that there is a minimiser of E_N on $(\overline{B}_{K_N})^N$, say \mathbf{X} . We want to prove that \mathbf{X} is actually a minimiser on all of \mathbb{R}^{Nd} . Let $\mathbf{X}' \in \mathbb{R}^{Nd}$. Necessarily, there exists $R \geq 0$ such that $\mathbf{X}' \in (\overline{B}_R)^N$. By Lemma 4.2 take a minimiser on $(\overline{B}_R)^N$, say \mathbf{Y} . We know that the diameter of \mathbf{Y} is less than or equal to K_N , so by possibly translating \mathbf{Y} (and by translation invariance of E_N) we may assume that $\mathbf{Y} \in (\overline{B}_{K_N})^N$ without loss of generality. Therefore $E_N(\mathbf{X}) \leq E_N(\mathbf{Y}) \leq E(\mathbf{X}')$, which shows, by the arbitrariness of the choice of \mathbf{X}' , that \mathbf{X} is a minimiser of E_N . This proves the first part of Theorem 4.1. The second part is straightforward: if $\mathbf{X} \in \mathbb{R}^{Nd}$ is a minimiser of E_N , then $\mathbf{X} \in (\overline{B}_R)^N$ for some $R \geq 0$, and so, by Lemma 4.2, its diameter is less than or equal to K_N . \blacksquare

4.2. Morrey-type regularity. This section is the discrete analogue of Section 3. As explained in the introduction, we define a discrete counterpart of the classical Morrey spaces of Definition 3.1.

Definition 4.3 (Empirical Morrey measures). Let $p \in [1, \infty]$ and $\mathbf{X} \in \mathbb{R}^{Nd}$. We say that $\mu_{\mathbf{X}}$ is an *empirical (or discrete) p -Morrey measure* if there exists $M > 0$ such that, for all $r > 0$ and $i \in \{1, \dots, N\}$,

$$m_{i,r}(\mathbf{X}) := \mu_{\mathbf{X}}(B_r(x_i)) - \frac{1}{N} \leq Mr^{d/q}, \quad (4.1)$$

where q is the Hölder dual of p . In this case we write $\mu_{\mathbf{X}} \in \mathcal{M}_p^N$, or simply $\mathbf{X} \in \mathcal{M}_p^N$. We also write

$$[\mu_{\mathbf{X}}]_{\mathcal{M}_p^N} = [\mathbf{X}]_{\mathcal{M}_p^N} := \sup \{r^{-d/q} m_{i,r}(\mathbf{X}) \mid (r, i) \in (0, \infty) \times \{1, \dots, N\}\}.$$

Given a configuration $\mathbf{X} = (x_1, \dots, x_N) \in \mathbb{R}^{Nd}$, throughout this paper we denote by $m_{i,r}(\mathbf{X})$ the total mass in the open ball of radius r centred at x_i , not counting the i th particle, as defined in (4.1). Note that, unlike $\|\cdot\|_{\mathcal{M}_p(\mathbb{R}^d)}$, $[\cdot]_{\mathcal{M}_p^N}$ does not define a norm; \mathcal{M}_p^N is not a Banach space or even a linear vector space.

We prove the following discrete regularity, an analogue of Theorem 3.2:

Theorem 4.4. *Suppose that W satisfies Hypothesis 1, it is β -repulsive with $0 < \beta < d$ and $\Delta^0 W \leq C_W$ for some $C_W > 0$. If $\mathbf{X} \in \mathbb{R}^{Nd}$ is a minimiser of the discrete interaction energy E_N , then $\mathbf{X} \in \mathcal{M}_p^N$ with $p = d/(d - \beta)$ and $[\mathbf{X}]_{\mathcal{M}_p^N} \leq C'$ for some $C' > 0$ only depending on W .*

The proof of Theorem 4.4 consists of the following three lemmas. The reader can follow the parallel with Section 3. The following notation is used throughout this paper: for any $r > 0$, $\mathbf{X} \in \mathbb{R}^{Nd}$ and $i \in \{1, \dots, N\}$, we write $S_{i,r}(\mathbf{X})$ to denote the set of indices of particles different from i which are at distance less than r from x_i , i.e.,

$$S_{i,r}(\mathbf{X}) := \{j \in \{1, \dots, N\} \mid j \neq i, |x_i - x_j| < r\} \quad (4.2)$$

and by $T_{i,r}(\mathbf{X})$ its complement, still removing i , that is,

$$T_{i,r}(\mathbf{X}) := \{j \in \{1, \dots, N\} \mid |x_i - x_j| \geq r\}. \quad (4.3)$$

Lemma 4.5. *Assume that W satisfies Hypothesis 1, and let $\mathbf{X} \in \mathbb{R}^{Nd}$ be a minimiser of E_N . Then*

$$\sum_{\substack{i=1 \\ i \neq j}}^N \Delta^0 W(x_i - x_j) \geq 0 \quad \text{for all } j \in \{1, \dots, N\}. \quad (4.4)$$

Proof. We write the minimiser $\mathbf{X} = (x_1, \dots, x_N)$. For all $j \in \{1, \dots, N\}$ define

$$p_j(x) := \frac{1}{N} \sum_{\substack{i=1 \\ i \neq j}}^N W(x_i - x) \quad \text{for all } x \in \mathbb{R}^d.$$

Consider $f_1: x \mapsto NE_N(x, x_2, \dots, x_N)$ and compute

$$f_1(x) = \frac{1}{N} \sum_{i=2}^N W(x_i - x) + \frac{1}{2N} \sum_{j=2}^N \sum_{\substack{i=2 \\ i \neq j}}^N W(x_i - x_j) = p_1(x) + \frac{1}{2N} \sum_{i=2}^N \sum_{\substack{i=2 \\ i \neq j}}^N W(x_i - x_j).$$

By the optimality of \mathbf{X} we know that x_1 is a minimiser of f_1 on \mathbb{R}^d . The very last term of the above computation is independent of x and therefore x_1 is also a minimiser of p_1 on \mathbb{R}^d . Hence $\Delta^0 p_1(x_1) \geq 0$. By repeating the above argument for all $j \geq 2$ we finally get $\Delta^0 p_j(x_j) \geq 0$ for all $j \in \{1, \dots, N\}$, which is the result. \blacksquare

Lemma 4.6. *Let W be as in Theorem 4.4 and let $\mathbf{X} \in \mathbb{R}^{Nd}$ be a minimiser of the discrete energy. There exists a constant $C' > 0$ (depending only on W) such that*

$$\frac{1}{N} \sum_{\substack{i=1 \\ i \neq j}}^N |x_i - x_j|^{-\beta} \leq C' \quad \text{for all } j \in \{1, \dots, N\}.$$

Proof. We prove it for $j = 1$ without loss of generality. Let δ and C be the constants appearing in the definition of β -repulsivity. In (4.4) we can separate the terms where the singularity of $\Delta^0 W$ is important to obtain

$$0 \leq \sum_{i=2}^N \Delta^0 W(x_i - x_1) \leq -C \sum_{i \in S_{1,\delta}(\mathbf{X})} |x_i - x_1|^{-\beta} + \sum_{i \in T_{1,\delta}(\mathbf{X})} \Delta^0 W(x_i - x_1)$$

$$\leq -C \sum_{i \in S_{1,\delta}(\mathbf{X})} |x_i - x_1|^{-\beta} + C_W N,$$

with the notation given in (4.2) and (4.3). This implies that $\sum_{i \in S_{1,\delta}(\mathbf{X})} |x_i - x_1|^{-\beta} \leq (C_W/C)N$, and consequently

$$\frac{1}{N} \sum_{i=2}^N |x_i - x_1|^{-\beta} = \frac{1}{N} \sum_{i \in S_{1,\delta}(\mathbf{X})} |x_i - x_1|^{-\beta} + \frac{1}{N} \sum_{i \in T_{1,\delta}(\mathbf{X})} |x_i - x_1|^{-\beta} \leq \frac{C_W}{C} + \delta^{-\beta},$$

which yields the result with $C' := C_W/C + \delta^{-\beta}$. \blacksquare

Lemma 4.7. *Let $0 < \beta < d$ and $\mathbf{X} \in \mathbb{R}^{Nd}$. Suppose that there is a constant $C' > 0$ with*

$$\frac{1}{N} \sum_{\substack{i=1 \\ i \neq j}}^N |x_i - x_j|^{-\beta} \leq C' \quad \text{for all } j \in \{1, \dots, N\}$$

Then $\mathbf{X} \in \mathcal{M}_p^N$ for $p = d/(d - \beta)$ and $[\mathbf{X}]_{\mathcal{M}_p^N} \leq C'$.

Proof. We want to prove that $m_{j,r}(\mathbf{X}) > C' r^\beta$ for all $r > 0$ and $j \in \{1, \dots, N\}$, with the notation in (4.1). Without loss of generality, assume $j = 1$. We have

$$r^{-\beta} m_{1,r}(\mathbf{X}) \leq \frac{1}{N} \sum_{i \in S_{1,r}(\mathbf{X})} |x_i - x_1|^{-\beta} \leq \frac{1}{N} \sum_{i=2}^N |x_i - x_1|^{-\beta} \leq C',$$

since $\beta > 0$, which is the result. \blacksquare

We give an additional lemma whose proof is analogous to that of Lemma 3.6 and we omit:

Lemma 4.8. *Let $p > 1$, $q = p/(p - 1)$ and $0 < \beta < d/q$. For all $r > 0$, there exists $C_r > 0$ (depending only on β , r , q and d) such that $C_r \rightarrow 0$ as $r \rightarrow \infty$ and, for all $\mathbf{X} \in \mathcal{M}_p^N$,*

$$\frac{1}{N} \sum_{i \in S_{j,r}} |x_i - x_j|^{-\beta} \leq C_r [\mathbf{X}]_{\mathcal{M}_p^N} \quad \text{for all } j \in \{1, \dots, N\},$$

where we refer the reader to the notation in (4.2).

Observe that, as for the continuum case in Section 3, Theorem 4.4 actually holds when $\mathbf{X} \in \mathbb{R}^{Nd}$ has finite energy and it is a local minimiser of the discrete energy since one can easily check that Lemma 4.5 stays true in this case. Local minimisers of the discrete energy are therefore discretely Morrey regular under the assumptions on W of Theorem 4.4.

4.3. Euler–Lagrange estimate. We prove an Euler–Lagrange estimate at the discrete level, as discussed in the introduction. It is the discrete analogue of the Euler–Lagrange equation given in the first line of (1.6). Recall that for every $\mathbf{X} \in \mathbb{R}^{Nd}$ we write

$$P_i(\mathbf{X}) := \frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^N W(x_i - x_j) \quad \text{for all } i \in \{1, \dots, N\}.$$

Note that $P_i(\mathbf{X}) = p_i(x_i)$, where p_i already appeared in the proof of Lemma 4.5.

Theorem 4.9. *Suppose that W satisfies Hypothesis 1–3 and let $\mathbf{X} \in \mathbb{R}^{Nd}$ be a minimiser of E_N . If W satisfies Hypothesis 3a, then*

$$|P_i(\mathbf{X}) - 2E_N(\mathbf{X})| \leq \frac{W(0) - W_{\min}}{N} \quad \text{for all } i \in \{1, \dots, N\}. \quad (4.5)$$

If W satisfies Hypothesis 3b, then there exist $A > 1$ and $k \in (0, 1]$ (independent of N and \mathbf{X}) such that

$$|P_i(\mathbf{X}) - 2E_N(\mathbf{X})| \leq AN^{-k} \quad \text{for all } i \in \{1, \dots, N\}.$$

One can take $k = 2/((\beta - 1)\beta)$.

Proof. First suppose that W satisfies Hypothesis 3a. We first prove

$$|P_i(\mathbf{X}) - P_j(\mathbf{X})| \leq \frac{W(0) - W_{\min}}{N} \quad \text{for all } i, j \in \{1, \dots, N\}. \quad (4.6)$$

To this end we proceed by contradiction by assuming that the result is not true. We move one particle of the minimiser at the exact location of another particle of the minimiser and show that the resulting energy is lower. With no loss of generality, suppose that $N(P_1(\mathbf{X}) - P_2(\mathbf{X})) > W(0) - W_{\min}$, and that we move x_1 at the location of x_2 . Write $\mathbf{X}' := (x_2, x_2, x_3, \dots, x_N)$ and compute

$$\begin{aligned} N^2(E_N(\mathbf{X}) - E_N(\mathbf{X}')) &= \sum_{i=2}^N W(x_1 - x_i) - \sum_{i=2}^N W(x_2 - x_i) \\ &= N(P_1(\mathbf{X}) - P_2(\mathbf{X})) - W(0) + W(x_1 - x_2) \\ &> W(0) - W_{\min} - W(0) + W_{\min} = 0, \end{aligned}$$

which is a contradiction to the fact that \mathbf{X} is a minimiser of E_N , and shows (4.6). Averaging (4.6) over $j = 1, \dots, N$ gives, for all $i \in \{1, \dots, N\}$,

$$\begin{aligned} \frac{W(0) - W_{\min}}{N} &\geq \frac{1}{N} \sum_{j=1}^N |P_i(\mathbf{X}) - P_j(\mathbf{X})| \\ &\geq \left| P_i(\mathbf{X}) - \frac{1}{N} \sum_{j=1}^N P_j(\mathbf{X}) \right| = |P_i(\mathbf{X}) - 2E_N(\mathbf{X})|, \end{aligned}$$

which shows (4.5).

Suppose now that W satisfies Hypothesis 3b. We first want to prove that, for some $A > 1$ and $k \in (0, 1]$,

$$|P_i(\mathbf{X}) - P_j(\mathbf{X})| \leq AN^{-k} \quad \text{for all } i, j \in \{1, \dots, N\}. \quad (4.7)$$

To this end we intend to reach a contradiction by assuming that

$$P_1(\mathbf{X}) - P_2(\mathbf{X}) > AN^{-k}$$

for some $N \geq 2$ arbitrarily large, and for some $A > 1$ and $k \in (0, 1]$ to be chosen appropriately later. We intend to reach a contradiction for certain values of A and k . We move the first particle of the minimiser, located at x_1 , to a point x'_2 close to the

second particle, located at x_2 . We want to show that, with an appropriate choice of x'_2 , the resulting energy is lower. Write $\mathbf{X}' := (x'_2, x_2, x_3, \dots, x_N)$ and compute

$$\begin{aligned}
2N^2(E_N(\mathbf{X}) - E_N(\mathbf{X}')) &= \sum_{i=2}^N W(x_1 - x_i) - \sum_{i=2}^N W(x'_2 - x_i) \\
&= N(P_1(\mathbf{X}) - P_2(\mathbf{X})) + \sum_{i=3}^N (W(x_2 - x_i) - W(x'_2 - x_i)) \\
&\quad - W(x'_2 - x_2) + W(x_2 - x_1) \\
&> AN^{1-k} + \sum_{i=3}^N (W(x_2 - x_i) - W(x'_2 - x_i)) \\
&\quad - W(x'_2 - x_2) + W_{\min}. \tag{4.8}
\end{aligned}$$

We need to bound from below the remaining terms involving W and show that they are strictly greater than $-AN^{1-k}$. To this end, x'_2 needs to be chosen carefully. We know by Lemma 4.6 that

$$\frac{1}{N} \sum_{\substack{i=1 \\ i \neq 2}}^N |x_i - x_2|^{-\beta} \leq C', \tag{4.9}$$

and in particular

$$|x_i - x_2| \geq (C'N)^{-1/\beta} = C_1N^{-1/\beta} \quad \text{for all } i \neq 2,$$

where $C_1 := (C')^{-1/\beta}$. Thus there are no other particles in a radius $C_1N^{-1/\beta}$ around x_2 . We pick x'_2 at less than half that distance to make sure that we stay away from other particles: we take

$$\alpha \geq 1/\beta, \tag{4.10}$$

to be chosen later, and pick x'_2 so that

$$2|x'_2 - x_2| = C_1N^{-\alpha} \leq C_1N^{-1/\beta} \leq |x_i - x_2| \quad \text{for all } i \neq 2. \tag{4.11}$$

Let us then bound the terms in (4.8) directly involving W . We have, by Hypothesis 3b and since N is large enough so that $C_1N^{-1/\beta}/2 \leq 1$,

$$W(x'_2 - x_2) \leq C_W|x'_2 - x_2|^{2-\beta} = C_W \left(\frac{C_1N^{-\alpha}}{2} \right)^{2-\beta} = C_2N^{\alpha(\beta-2)},$$

where $C_2 := C_W(C_1/2)^{2-\beta}$. Since we need this to be smaller than AN^{1-k} , we impose $k = 1 - \alpha(\beta - 2)$, so that

$$W(x'_2 - x_2) \leq C_2N^{1-k}. \tag{4.12}$$

For the other term, pick a cut-off distance $\ell = \ell(N) < 1/3$, to be chosen later, and let

$$S := S_{2,\ell}(\mathbf{X}) \setminus \{1\},$$

where we refer the reader to the notation given in (4.2). We write

$$\begin{aligned} \left| \sum_{i=3}^N (W(x_2 - x_i) - W(x'_2 - x_i)) \right| &\leq \sum_{\substack{i=3 \\ i \notin S}}^N |W(x_2 - x_i) - W(x'_2 - x_i)| \\ &\quad + \sum_{i \in S} |W(x_2 - x_i)| + \sum_{i \in S} |W(x'_2 - x_i)|. \end{aligned} \quad (4.13)$$

The next-to-last term can be estimated, using (4.9) and Hypothesis 3b, as

$$\begin{aligned} \frac{1}{N} \sum_{i \in S} |W(x_2 - x_i)| &\leq \frac{C_W}{N} \sum_{i \in S} |x_2 - x_i|^{2-\beta} \\ &\leq C_W \left(\frac{1}{N} \sum_{i \in S} |x_2 - x_i|^{-\beta} \right)^{(\beta-2)/\beta} \left(\frac{|S|}{N} \right)^{2/\beta} \\ &\leq C_W (C')^{(\beta-2)/\beta} \left(\frac{|S|}{N} \right)^{2/\beta} = C_3 \left(\frac{|S|}{N} \right)^{2/\beta}, \end{aligned}$$

where $C_3 := C_W (C')^{(\beta-2)/\beta}$. On the other hand, due to Lemma 4.7, we have

$$\frac{|S|}{N} \leq C' \ell^\beta.$$

Hence

$$\sum_{i \in S} |W(x_2 - x_i)| \leq C_3 (C')^{2/\beta} \ell^2 N = C_4 \ell^2 N,$$

where $C_4 := C_3 (C')^{2/\beta}$. This motivates the choice $\ell := N^{-k/2}$ which is less than $1/3$ for N large enough, so that

$$\sum_{i \in S} |W(x_2 - x_i)| \leq C_4 N^{1-k}. \quad (4.14)$$

The last term in (4.13) is comparable to the one we just bounded, since $|x_i - x_2|$ and $|x_i - x'_2|$ are comparable due to (4.11). Indeed,

$$|x_i - x_2| \leq |x_i - x'_2| + |x'_2 - x_2| = |x_i - x'_2| + \frac{1}{2}|x_i - x_2|,$$

so that

$$|x_i - x_2| \leq 2|x_i - x'_2|.$$

With this, and what we proved above,

$$\sum_{i \in S} |W(x'_2 - x_i)| \leq C_W \sum_{i \in S} |x'_2 - x_i|^{2-\beta} \leq 2^{\beta-2} C_W \sum_{i \in S} |x_2 - x_i|^{2-\beta} \leq C_5 N^{1-k}, \quad (4.15)$$

where $C_5 := 2^{\beta-2} C_W C_4$. Finally, for the first term in (4.13), notice that for $i \in S$ we have $|x_2 - x_i| \leq \ell$ (by definition of S), and also

$$|x'_2 - x_i| \leq |x'_2 - x_2| + |x_2 - x_i| \leq \frac{1}{2}|x_2 - x_i| + |x_2 - x_i| \leq \frac{3}{2}\ell$$

due to (4.11). Since we are requiring $\ell < 1/3$, both $x_2 - x_i$ and $x'_2 - x_i$ are in the ball of radius 1 centred at 0 and we may use the gradient bound in Hypothesis 3b to get

$$\begin{aligned} \sum_{\substack{i=3 \\ i \notin S}}^N |W(x_2 - x_i) - W(x'_2 - x_i)| &\leq C_W N \ell^{1-\beta} |x_2 - x'_2| \\ &\leq \frac{C_1}{2} C_W N \ell^{1-\beta} N^{-\alpha} = C_6 N^{1+k(\beta-1)/2-\alpha}, \end{aligned} \quad (4.16)$$

where $C_6 := C_1 C_W / 2$, thanks to (4.11). Since $\alpha(\beta - 2) = 1 - k$, choose k so that $1 + k(\beta - 1)/2 - (1 - k)/(\beta - 2) = 1 - k$, that is,

$$k := \frac{2}{(\beta - 1)\beta}.$$

This gives

$$\alpha = \frac{1 - k}{\beta - 2} = \frac{\beta + 1}{(\beta - 1)\beta} \geq \frac{1}{\beta},$$

as required in (4.10). Putting together (4.8), (4.12), (4.13), (4.14), (4.15) and (4.16),

$$2N^2 (E_N(\mathbf{X}) - E_N(\mathbf{X}')) > (A - C_2 - C_4 - C_5 - C_6) N^{1-k} + W_{\min}.$$

An appropriate choice of the constant A makes this quantity positive for all N large enough, contradicting the fact that \mathbf{X} is a minimiser of E_N , thus showing (4.7).

Averaging (4.7) over $j = 1, \dots, N$ we get, for all $i \in \{1, \dots, N\}$,

$$\frac{A}{N^k} \geq \frac{1}{N} \sum_{j=1}^N |P_i(\mathbf{X}) - P_j(\mathbf{X})| \geq \left| P_i(\mathbf{X}) - \frac{1}{N} \sum_{j=1}^N P_j(\mathbf{X}) \right| = |P_i(\mathbf{X}) - 2E_N(\mathbf{X})|,$$

which ends the proof. ■

4.4. Diameter estimates. As a tool to prove our main result we need to introduce the following notion of discrete instability:

Definition 4.10 (Discrete instability). Let $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ and suppose that $W_\infty := \lim_{|x| \rightarrow \infty} W(x)$ exists (possibly $+\infty$). We say that W is *discretely unstable* (with constant $s > 0$) if there exist $s > 0$ and $\bar{N} \geq 2$ such that, for all $N > \bar{N}$, there exists $\mathbf{X} \in \mathbb{R}^{Nd}$ with

$$E_N(\mathbf{X}) < \frac{1}{2} W_\infty - s.$$

Note that if W is discretely unstable with some constant s , then it is so with any $s' < s$. This definition is a natural discrete version of the instability in Definition 1.1, and it is the one we need in order to carry out the next arguments. Actually, both concepts turn out to be equivalent under Hypotheses 1–3; see Proposition 5.4.

Lemma 4.11. *Assume that W satisfies Hypotheses 1–3 and is discretely unstable. There exist $\bar{N} \geq 2$ and $r, m > 0$ depending only on W such that, for each $N > \bar{N}$ and any minimiser \mathbf{X} of E_N on \mathbb{R}^{Nd} it holds that*

$$m_{i,r}(\mathbf{X}) \geq m \quad \text{for all } i \in \{1, \dots, N\},$$

where we use the notation in (4.1).

Proof. Suppose first that W satisfies Hypothesis 3a. Let \mathbf{X} be a minimiser of E_N and write $E_N^0 := E_N(\mathbf{X})$. Then, by Theorem 4.9, for all $i \in \{1, \dots, N\}$,

$$P_i(\mathbf{X}) \leq 2E_N^0 + \frac{W(0) - W_{\min}}{N}.$$

Let $s > 0$ be the constant in the definition of discrete instability. We can pick $\bar{N} \geq 2$ such that, for all $N > \bar{N}$, $E_N^0 < W_\infty/2 - s$. Thus,

$$E_0 := \sup_{N \geq \bar{N}} E_N^0 \leq \frac{1}{2}W_\infty - s < \frac{1}{2}W_\infty.$$

Let $\rho \in \mathcal{P}(\mathbb{R}^d)$ be such that $E(\rho) < +\infty$, which exists by local integrability of W . By Lemma 5.3 there exists a sequence of particle configurations $(\mathbf{X}_N^*)_{N \geq 2}$ such that

$$\limsup_{N \rightarrow \infty} E_N^0 \leq \lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*) = E(\rho) < +\infty,$$

so that E_0 is finite even if W_∞ is not. We can then take a such that $W_{\min}/2 \leq E_0 < a < W_\infty/2$. Let $r > 0$ be such that $W(x) > 2a$ for all $|x| > r$. Compute, for all $N > \bar{N}$,

$$\begin{aligned} 2E_0 + \frac{W(0) - W_{\min}}{N} &\geq P_i(\mathbf{X}) = \frac{1}{N} \sum_{j \in S_{i,r}(\mathbf{X})} W(x_i - x_j) + \frac{1}{N} \sum_{j \in T_{i,r}(\mathbf{X})} W(x_i - x_j) \\ &\geq W_{\min} m_{i,r}(\mathbf{X}) + \frac{2a}{N} \sum_{j \in T_{i,r}(\mathbf{X})} 1 \\ &= W_{\min} m_{i,r}(\mathbf{X}) + 2a \left(1 - m_{i,r}(\mathbf{X}) - \frac{1}{N} \right) \\ &= (W_{\min} - 2a) m_{i,r}(\mathbf{X}) + 2a \left(1 - \frac{1}{N} \right), \end{aligned}$$

where the notation is as in (4.2) and (4.3). Since $W_{\min} < 2a$ we get

$$m_{i,r}(\mathbf{X}) \geq \frac{2E_0 - 2a + N^{-1}(W(0) - W_{\min} + 2a)}{W_{\min} - 2a}.$$

Since $E_0 < a$, there exists $b > 0$ such that $b < 2a - 2E_0$. Then, for some number of particles large enough, which we still denote by \bar{N} , we have $(W(0) - W_{\min} + 2a)/N < 2a - 2E_0 - b$ for all $N > \bar{N}$. Therefore,

$$m_{i,r}(\mathbf{X}) \geq \frac{-b}{W_{\min} - 2a} =: m > 0 \quad \text{for all } N > \bar{N}.$$

The choices of a and b only depend on W and therefore r and m only depend on W as well, which shows the result when Hypothesis 3a holds.

If now W satisfies Hypothesis 3b, then the arguments above can still be carried out in the same fashion using the second part of Theorem 4.9 instead of the first. \blacksquare

Theorem 4.12. *Assume that W satisfies Hypotheses 1–3 and it is discretely unstable. There is a constant $K > 0$ depending only on W (in particular, independent of N) such that the diameter of any discrete minimiser is less than K .*

Proof. Let $\bar{N} \geq 2$, m and r be as in Lemma 4.11, and let $\mathbf{X} \in \mathbb{R}^{Nd}$ be a minimiser of E_N for some $N > \bar{N}$. We can carry out an argument along the same lines as in the proof of [12, Lemma 2.9]. We briefly explain the idea: due to Lemma 4.11, in a ball of radius r around each x_i there are at least mN other particles; hence there exist $\ell \leq \lceil 1/m \rceil$ indices i_1, \dots, i_ℓ (where $\lceil \cdot \rceil$ is the ceiling function) such that

$$\{x_1, \dots, x_N\} \subset B_{2r}(x_{i_1}) \cup \dots \cup B_{2r}(x_{i_\ell}),$$

and such that the balls $B_r(x_{i_1}), \dots, B_r(x_{i_\ell})$ are disjoint. Now, relabel the points $x_{i_1}, \dots, x_{i_\ell}$ so that they are ordered according to their first coordinate. Following the same argument as in Lemma 4.2 we see that

$$|\pi_1(x_{i_k}) - \pi_1(x_{i_{k+1}})| \leq 4r + 2R_W \quad \text{for all } k \in \{1, \dots, \ell - 1\},$$

where R_W is the constant in Hypothesis 2 (otherwise one can slightly shorten the gap in the first coordinate and decrease the energy). This shows that the diameter of the projection of the set $\{x_1, \dots, x_N\}$ in the first coordinate is not larger than $2(\lceil 1/m \rceil - 1)(2r + R_W) + 4r$. As the argument can be repeated for all projections, we deduce that

$$\text{diam } \mathbf{X} \leq 2\sqrt{d}(\lceil 1/m \rceil - 1)(2r + R_W) + 4r =: K_1.$$

This holds for any $N > \bar{N}$. Since for $N \leq \bar{N}$ the diameter of minimisers is bounded by $K_2 := 2\sqrt{d}(\bar{N} - 1)R_W$ by Theorem 4.1, we obtain the result for $K := \max\{K_1, K_2\}$. ■

5. MANY-PARTICLE LIMIT

In this section we complete the proof of Theorem 1.2.

5.1. Convergence of discrete minimisers. We show that if the potential W is unstable then any sequence of discrete minimisers has a subsequence which converges in the narrow topology (up to translations) to a continuum minimiser as $N \rightarrow \infty$.

We first prove the following:

Lemma 5.1. *Let W satisfy Hypotheses 1–3 and let it be discretely unstable. Then any sequence $(\mathbf{X}_N)_{N \geq 2}$ of discrete minimisers converges, up to a subsequence and to translations, to some $\rho \in \mathcal{P}(\mathbb{R}^d)$.*

Proof. Let $(\mathbf{X}_N)_{N \geq 2}$ be a sequence such that \mathbf{X}_N is a minimiser of E_N for all $N \geq 2$. The diameter of \mathbf{X}_N is uniformly bounded by the constant K in Theorem 4.12. Since E_N is translation invariant there exists a sequence of minimisers of E_N , which we still denote by $(\mathbf{X}_N)_{N \geq 2}$, obtained by suitable translations of the original sequence and such that $\mathbf{X}_N \in (B_K)^{\bar{N}}$ for all $N \geq 2$. Then, since K is independent of N we can extract a subsequence of $(\mathbf{X}_N)_{N \geq 2}$ converging in the narrow topology to a $\rho \in \mathcal{P}(\mathbb{R}^d)$. ■

In order to complete the proof of Theorem 1.2(1) we need to show that instability (Definition 1.1) implies discrete instability (Definition 4.10). In fact, we show that they are both equivalent under Hypotheses 1–3. We also take the opportunity to compare them to the concept of H -stability found in statistical mechanics (see for example [43, Definition 3.2.1]). We actually define H -instability, which is its complementary:

Definition 5.2 (H -instability). Let $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ and suppose that $W_\infty := \lim_{|x| \rightarrow \infty} W(x)$ exists (possibly $+\infty$). We say that W is H -unstable if, for all $B \in \mathbb{R}$, there exist $N \geq 2$ and $\mathbf{X} \in \mathbb{R}^{Nd}$ with

$$E_N(\mathbf{X}) < \frac{1}{2}W_\infty - \frac{B}{2N}.$$

The proposition below shows that there is equivalence among instability, discrete instability and H -instability if Hypotheses 1, 2 and 3a hold; equivalence between H -instability and instability if Hypothesis 3a holds was already proved in [45]. If Hypotheses 1, 2 and 3b hold (so that a singularity of the potential at $x = 0$ is allowed), then we only have that instability and discrete instability are equivalent and that they imply H -instability. Whether the converse implication is true or not in this case is an open question. By the proof of Proposition 5.4 one sees that the main difficulty when W is unbounded is that we cannot take $B = W(0)$ in the Definition of H -instability; therefore, what we can prove by our approach is only that H -instability implies the complementary of strict stability.

A word on the terminology is in order: we have chosen Definitions 1.1 and 4.10 so as to maintain agreement with “instability” in the statistical mechanics literature as, for example, in [5]. More importantly, we have wanted to keep “stable” as the opposite concept of “unstable”, which due to the equivalences above determines a natural definition. Unfortunately, this terminology leaves us without a good term to say “there exists $\rho \in \mathcal{P}(\mathbb{R}^d)$ with $E(\rho) \leq W_\infty/2$ ”, that is, to say “ W is not strictly stable”.

In order to compare the concepts of stability we need to use a good discrete approximation to a given measure ρ . We give it in the following lemma, whose proof is postponed to Section 6. The following result actually implies the Γ -convergence of the discrete energy to the continuum one; we refer to Section 6 for details on this.

Lemma 5.3. *Assume that the potential W satisfies Hypotheses 1–3.*

- (1) *All sequences $(\mathbf{X}_N)_{N \geq 2}$ with $\mathbf{X}_N \in \mathbb{R}^{Nd}$ for all $N \geq 2$ such that $\mu_{\mathbf{X}_N} \rightharpoonup \rho$ in the narrow topology as $N \rightarrow \infty$ for some $\rho \in \mathcal{P}(\mathbb{R}^d)$ satisfy*

$$E(\rho) \leq \liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N).$$

- (2) *Let $\rho \in \mathcal{P}(\mathbb{R}^d)$ if Hypothesis 3a holds, or $\rho \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d-\beta)$ if Hypothesis 3b holds. There exists a sequence $(\mathbf{X}_N^*)_{N \geq 2}$ with $\mathbf{X}_N^* \in \mathbb{R}^{Nd}$ for all $N \geq 2$ such that $\mu_{\mathbf{X}_N^*} \rightharpoonup \rho$ in the narrow topology as $N \rightarrow \infty$ and*

$$E(\rho) = \lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*).$$

(We refer to this subsequence as a recovery sequence for ρ .)

Using this approximation result and Lemma 5.1 we can show the following:

Proposition 5.4. *Suppose that W satisfies Hypotheses 1–3 and $W_\infty := \lim_{|x| \rightarrow \infty} W(x)$ exists (possibly $+\infty$). If Hypothesis 3a holds, then we have:*

$$W \text{ is unstable} \iff W \text{ is discretely unstable} \iff W \text{ is } H\text{-unstable.} \quad (5.1)$$

If Hypotheses 1, 2 and 3b hold, then we have:

$$W \text{ is unstable} \iff W \text{ is discretely unstable} \implies W \text{ is } H\text{-unstable.} \quad (5.2)$$

Proof. Let W satisfy Hypothesis 3a. In this case the fact that instability is equivalent to H -instability was already proved in [45, Proposition 4.1]. We therefore only have to prove that instability is equivalent to discrete instability. Suppose first that W is unstable and let $\rho \in \mathcal{P}(\mathbb{R}^d)$ be such that $E(\rho) < W_\infty/2$. Then, by Lemma 5.3(2),

$$\lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*) = E(\rho) < \frac{1}{2}W_\infty,$$

where \mathbf{X}_N^* is a recovery sequence for ρ . Therefore there exists $s > 0$ such that $E_N(\mathbf{X}_N^*) < W_\infty/2 - s$ for all N large enough, which proves that W is discretely unstable. Suppose now that W is discretely unstable. Then there exist $s > 0$ and $\bar{N} \geq 2$ such that, for each $N > \bar{N}$, we can choose $\mathbf{X} \in \mathbb{R}^{Nd}$ with $E_N(\mathbf{X}) < W_\infty/2 - s$ and $s > W(0)/(2N)$. Hence

$$E(\mu_{\mathbf{X}}) = E_N(\mathbf{X}) + \frac{W(0)}{2N} < \frac{1}{2}W_\infty - s + \frac{W(0)}{2N} < \frac{1}{2}W_\infty,$$

which ends the proof of (5.1).

Let now W satisfy Hypotheses 1, 2 and 3b. Suppose that W is unstable. Then we know by [12, Theorem 1.4] and Theorem 3.2 that there exists a minimiser $\rho \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ of E with $p = d/(d - \beta)$. As above, Lemma 5.3(2) gives us that W is discretely unstable. Let W be discretely unstable, so that there exist $s > 0$ and $\bar{N} \geq 2$ such that, for each $N > \bar{N}$ we can choose $\mathbf{X} \in \mathbb{R}^{Nd}$ with $E_N(\mathbf{X}) < W_\infty/2 - s$. Then, by Theorem 4.1, there exists a minimiser \mathbf{X}_N of E_N for every $N > \bar{N}$ such that $E_N(\mathbf{X}_N) < W_\infty/2 - s$. By Lemma 5.1 the sequence $(\mathbf{X}_N)_{N \geq 2}$ converges, up to a subsequence and to translations, to some $\rho \in \mathcal{P}(\mathbb{R}^d)$, and Lemma 5.3(1) gives us

$$E(\rho) \leq \liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) \leq \frac{1}{2}W_\infty - s < \frac{1}{2}W_\infty,$$

which shows that W is unstable. Also, for every $B \in \mathbb{R}$ there exists $N \geq 2$ large enough such that $B/(2N) < s$ which proves that, for such N ,

$$E_N(\mathbf{X}) < \frac{1}{2}W_\infty - s < \frac{1}{2}W_\infty - \frac{B}{2N},$$

where \mathbf{X} is as above. This ends the proof of (5.2). \blacksquare

We end this section with the following lemma, which finally shows Theorem 1.2(1):

Lemma 5.5. *Let W satisfy Hypotheses 1–3 and let it be unstable. Then any sequence $(\mathbf{X}_N)_{N \geq 2}$ of discrete minimisers converges, up to a subsequence and to translations, to some $\rho \in \mathcal{P}(\mathbb{R}^d)$. Furthermore, ρ is a continuum minimiser.*

Proof. Let $(\mathbf{X}_N)_{N \geq 2}$ be a sequence such that \mathbf{X}_N is a minimiser of E_N for all $N \geq 2$. By Proposition 5.4 and Lemma 5.1 we know that $(\mathbf{X}_N)_{N \geq 2}$ converges, up to a subsequence and to translations, to some $\rho \in \mathcal{P}(\mathbb{R}^d)$.

Let us prove that ρ is a minimiser of E . Take $\nu \in \mathcal{P}(\mathbb{R}^d)$ if W satisfies Hypothesis 3a, and $\nu \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d - \beta)$ if W satisfies Hypothesis 3b. We know by Lemma 5.3(2) that there is a recovery sequence $(\mathbf{X}_N^*)_{N \geq 2}$ for ν . Lemma 5.3 and the minimality of the sequence $(\mathbf{X}_N)_{N \geq 2}$ lead to

$$E(\nu) = \lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*) \geq \lim_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq \liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq E(\rho),$$

which ends the proof, since, by [12, Theorem 1.4] and Theorem 3.2, if W satisfies Hypothesis 3b then minimisers of E exist and belong to $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d - \beta)$. ■

5.2. Unbounded growth of the diameter. We show that if the potential W is strictly stable, then the diameter of any sequence of discrete minimisers must diverge; that is, we prove Theorem 1.2(2).

We first prove that Morrey regularity is preserved under the narrow limit. This actually further motivates the notion of discrete Morrey measures as in Definition 4.3.

Lemma 5.6. *Let $(\mathbf{X}_N)_{N \geq 2}$ be a sequence of configurations converging narrowly to some $\rho \in \mathcal{P}(\mathbb{R}^d)$. Let $p \in [1, \infty]$ and suppose that there exists $M > 0$ such that $[\mathbf{X}_N]_{\mathcal{M}_p^N} \leq M$ for all $N \geq 2$. Then $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ and $\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} \leq 2^{d/q}M$, with q the Hölder dual of p .*

Proof. Take any integer $N \geq 2$, $x \in \mathbb{R}^d$ and $r > 0$, and write $\mathbf{X}_N = (x_1, \dots, x_N)$. Assume that there is $i \in \{1, \dots, N\}$ such that $x_i \in B_r(x)$. Since $B_r(x) \subset B_{2r}(x_i)$, using that $\mathbf{X}_N \in \mathcal{M}_p^N$ with $[\mathbf{X}_N]_{\mathcal{M}_p^N} \leq M$ we have

$$\mu_{\mathbf{X}_N}(B_r(x)) \leq \mu_{\mathbf{X}_N}(B_{2r}(x_i)) \leq \frac{1}{N} + M(2r)^{d/q}.$$

On the other hand, if there is no $i \in \{1, \dots, N\}$ such that $x_i \in B_r(x)$ then the previous inequality holds trivially. By the Portmanteau theorem (see for example [7, Theorem 2.1]), taking limits as $N \rightarrow \infty$ gives the result:

$$\rho(B_r(x)) \leq \liminf_{N \rightarrow \infty} \mu_{\mathbf{X}_N}(B_r(x)) \leq 2^{d/q}Mr^{d/q}. \quad \blacksquare$$

We conclude by the following lemma:

Lemma 5.7. *Let W satisfy Hypotheses 1–3 and let it be strictly stable. Then any sequence $(\mathbf{X}_N)_{N \geq 2}$ of discrete minimisers is such that $\text{diam } \mathbf{X}_N \rightarrow \infty$ as $N \rightarrow \infty$.*

Proof. Let $(\mathbf{X}_N)_{N \geq 2}$ be a sequence of discrete minimisers. If $\text{diam } \mathbf{X}_N$ does not diverge one can find, after suitable translations of $(\mathbf{X}_N)_{N \geq 2}$ (by translation invariance of E_N), a sequence of minimisers which are uniformly compactly supported. By compactness we can extract a subsequence converging in the narrow topology to some $\rho \in \mathcal{P}(\mathbb{R}^d)$.

Let W first satisfy Hypothesis 3a. Then, by the same argument as in the proof of Lemma 5.5, ρ must be a continuum minimiser. But we know that continuum minimisers do not exist if W is strictly stable due to [12, Theorem 3.3] and [45, Theorem 3.2], so we have reached a contradiction. We deduce that $\text{diam } \mathbf{X}_N$ diverges.

If now W satisfies Hypothesis 3b, then $\mathbf{X}_N \in \mathcal{M}_p^N$ with $p = d/(d - \beta)$ for all $N \geq 2$, by Theorem 4.4, and so $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ by Lemma 5.6. The same argument as in the proof of Lemma 5.5 gives us that ρ is a minimiser of E on $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$. This is again a contradiction since the results in [12, 45] actually show that there are no minimisers on $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ if W is strictly stable; indeed one can construct a sequence $(\rho_n)_{n \in \mathbb{N}}$ in $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ such that $E(\rho_n) \rightarrow W_\infty/2$ as $n \rightarrow \infty$, which contradicts the strict stability of W if a minimiser on $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ exists. (The sequence ρ_n can be chosen to be the uniform probability on the ball of radius n ; see [12, Theorem 3.3].) ■

6. Γ -CONVERGENCE OF THE DISCRETE ENERGY

In this section we derive a constructive way of approximating an element of $\mathcal{P}(\mathbb{R}^d)$ by a sequence of empirical measures. We show that this way of constructing an approximating sequence actually gives rise to a recovery sequence with respect to our discrete and continuum energies (1.1) and (1.2), respectively. That is: given a measure $\rho \in \mathcal{P}(\mathbb{R}^d)$ we can approximate it narrowly by N -particle empirical measures in such a way that their discrete interaction energy also approximates the continuum interaction energy of ρ . Thus we prove Lemma 5.3 which was used in the previous section. This approximation property is contained in the notion of Γ -convergence, which we give with respect to the narrow topology. Recall that the narrow topology on $\mathcal{P}(\mathbb{R}^d)$ is, by definition, obtained by duality with the space of continuous bounded functions on \mathbb{R}^d . By the Portmanteau theorem (see [7, Theorem 2.1]) it can actually be equivalently obtained by duality with the space of Lipschitz bounded functions on \mathbb{R}^d ; this is a property which we use later on. Also, the narrow topology can be metrised by, for example, the Lévy–Prokhorov distance; see [47, Section 6] for the definition and other examples of distances metrising the narrow topology. If we restrict ourselves to elements in $\mathcal{P}(\mathbb{R}^d)$ which have finite p th moment for some $p \in [1, \infty)$, then it can also be metrised by the Wasserstein distance of order p ; see [2, 47]. In the following we denote by σ any of these metrising distances.

Definition 6.1 (Γ -convergence). Let A be a subset of $\mathcal{P}(\mathbb{R}^d)$. We say that the discrete energy $(E_N)_{N \geq 2}$ Γ -converges (narrowly) to the continuum energy E on A if the following two inequalities are met for all $\rho \in A$.

- (i) (liminf inequality) All sequences $(\mathbf{X}_N)_{N \geq 2}$ with $\mathbf{X}_N \in \mathbb{R}^{Nd}$ for all $N \geq 2$ such that $\sigma(\mu_{\mathbf{X}_N}, \rho) \rightarrow 0$ as $N \rightarrow \infty$ satisfy $E(\rho) \leq \liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N)$.
- (ii) (limsup inequality) There exists a sequence $(\mathbf{X}_N^*)_{N \geq 2}$ with $\mathbf{X}_N^* \in \mathbb{R}^{Nd}$ for all $N \geq 2$ such that $\sigma(\mu_{\mathbf{X}_N^*}, \rho) \rightarrow 0$ as $N \rightarrow \infty$ and $E(\rho) \geq \limsup_{N \rightarrow \infty} E_N(\mathbf{X}_N^*)$. Such a sequence is called a *recovery sequence* for ρ .

A sequence $(\mathbf{X}_N^*)_{N \geq 2}$ as in the limsup inequality is called a recovery sequence for ρ because one can check that $E_N(\mathbf{X}_N^*) \rightarrow E(\rho)$ as $N \rightarrow \infty$. The notion of Γ -convergence arises naturally in the discrete approximation of minimisers of energy functionals because, along with compactness, it ensures that a sequence of discrete minimisers converges to a minimiser of the continuum energy. (A continuum minimiser thus exists.) Formally, if $(\mathbf{X}_N)_{N \geq 2}$ is a sequence of minimisers of E_N and there exists $\rho \in \mathcal{P}(\mathbb{R}^d)$ such that $\sigma(\mu_{\mathbf{X}_N}, \rho) \rightarrow 0$ as $N \rightarrow \infty$ up to a subsequence, then the Γ -convergence of E_N to E on a set A implies: for any $\nu \in A$ there exists $(\mathbf{Y}_N)_{N \geq 2}$ such that

$$E(\nu) \geq \limsup_{N \rightarrow \infty} E_N(\mathbf{Y}_N) \geq \limsup_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq \liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq E(\rho),$$

which shows that ρ is a minimiser of E on A . This is a fundamental theorem of Γ -convergence which we already used in the proof of Lemma 5.5. For a detailed introduction to Γ -convergence we refer the reader to [8, 24]. We now show the Γ -convergence of E_N to E .

Theorem 6.2. *Assume W satisfies Hypotheses 1–3.*

- (1) If Hypothesis 3a holds, then $(E_N)_{N \geq 2}$ Γ -converges to E on $\mathcal{P}(\mathbb{R}^d)$.
- (2) If Hypothesis 3b holds, then $(E_N)_{N \geq 2}$ Γ -converges to E on $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d - \beta)$.

In the rest of this section we prove Theorem 6.2; in fact, we prove the slightly stronger statement given in Lemma 5.3. (The liminf inequality holds indeed on all of $\mathcal{P}(\mathbb{R}^d)$ even when Hypothesis 3b holds; see Remark 6.4.) We first show the liminf inequality and then the limsup inequality of Definition 6.1.

We use the following lemma whose proof can be found in [12, Lemma 2.1]:

Lemma 6.3. *If $W: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{-\infty, +\infty\}$ is a measurable function which is bounded from below (resp. above) and lower (resp. upper) semicontinuous, then E as defined in (1.2) is narrowly lower (resp. upper) semicontinuous.*

6.1. Liminf inequality. Let $\rho \in \mathcal{P}(\mathbb{R}^d)$ and $(\mathbf{X}_N)_{N \geq 2}$ be such that $\sigma(\mu_{\mathbf{X}_N}, \rho) \rightarrow 0$ as $N \rightarrow \infty$. Suppose first that W satisfies Hypothesis 3a. Then $W(0)$ is finite and

$$\liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) = \liminf_{N \rightarrow \infty} \left(E(\mu_{\mathbf{X}_N}) - \frac{W(0)}{2N} \right) \geq E(\rho),$$

by narrow lower semicontinuity of E , by Lemma 6.3, which is the result.

Now, suppose that W satisfies Hypothesis 3b; then $W(0) = +\infty$. Assume that $\liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) < +\infty$ or we are done. Let $\{W_\varepsilon\}_{\varepsilon > 0}$ be a family of potentials such that $W_\varepsilon(x) = W(x)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $W_\varepsilon(0) = 1/\varepsilon$ for all $\varepsilon > 0$. So defined, W_ε is lower semicontinuous; E_ε , defined by $E_\varepsilon(\nu) := 2^{-1} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W_\varepsilon(x - y) d\nu(x) d\nu(y)$ for all $\nu \in \mathcal{P}(\mathbb{R}^d)$, is therefore narrow lower semicontinuous by Lemma 6.3. Define $E_N^\varepsilon(\mathbf{X}_N) := (2N^2)^{-1} \sum_{i=1}^N \sum_{j=1, j \neq i}^N W_\varepsilon(x_i - x_j)$, where $\mathbf{X}_N = (x_1, \dots, x_N)$. Then $E_N^\varepsilon(\mathbf{X}_N) \leq E_N(\mathbf{X}_N)$ for all $\varepsilon > 0$ and

$$\liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq \liminf_{N \rightarrow \infty} E_N^\varepsilon(\mathbf{X}_N) = \liminf_{N \rightarrow \infty} \left(E_\varepsilon(\mu_{\mathbf{X}_N}) - \frac{W_\varepsilon(0)}{2N} \right) \geq E_\varepsilon(\rho). \quad (6.1)$$

We now need to show that $E_\varepsilon(\rho) \rightarrow E(\rho)$ as $\varepsilon \rightarrow 0$. If ρ has no atomic part, then $E_\varepsilon(\rho) = E(\rho)$ and we are done. We want to show by contradiction that ρ cannot have an atomic part. If ρ has an atomic part $\alpha \delta_z$ for some $0 < \alpha \leq 1$ and $z \in \mathbb{R}^d$, then, by boundedness from below of W ,

$$\begin{aligned} 2E_\varepsilon(\rho) &\geq \alpha^2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W_\varepsilon(x - y) d\delta_z(x) d\delta_z(y) + W_{\min}(1 - \alpha^2) \\ &= \frac{\alpha^2}{\varepsilon} + W_{\min}(1 - \alpha^2) \xrightarrow{\varepsilon \rightarrow 0} +\infty. \end{aligned}$$

This contradicts (6.1) and the fact that $\liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) < +\infty$. Therefore ρ cannot have an atomic part and we get the result:

$$\liminf_{N \rightarrow \infty} E_N(\mathbf{X}_N) \geq E(\rho).$$

Remark 6.4. The computations above tell us that the liminf inequality is actually true on all of $\mathcal{P}(\mathbb{R}^d)$ even if Hypothesis 3b holds; ρ does not need to be Morrey regular in the above proof. Hence the liminf inequality is true not only on $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ (as stated in Theorem 6.2), but also on $\mathcal{P}(\mathbb{R}^d)$ (as stated in Lemma 5.3).

6.2. Limsup inequality. We first assume that $\rho \in \mathcal{P}(\mathbb{R}^d)$ is compactly supported and then we extend the result to noncompactly supported probability measures by a density argument in Section 6.2.4. We need to construct a sequence of particle configurations that approximates ρ narrowly and whose discrete energy approximates the continuum energy of ρ .

6.2.1. Construction of the approximation. The construction presented here is inspired by [45, Proposition 4.1]. Fix any $N \geq 2$ and suppose that $\text{supp } \rho \subset [-L, L]^d$ for some $L \geq 1$. Call $n := \lfloor N^{1/(4d)} \rfloor \geq 1$, where $\lfloor \cdot \rfloor$ denotes the integer part, and divide the interval $[-L, L]$ into n equal subintervals of length $2L/n$, which gives a subdivision of $[-L, L]^d$ into n^d equal cubes of the form

$$\left[-L + \frac{2i_1 L}{n}, -L + \frac{2(i_1 + 1)L}{n} \right) \times \cdots \times \left[-L + \frac{2i_d L}{n}, -L + \frac{2(i_d + 1)L}{n} \right),$$

for $(i_1, \dots, i_d) \in \{0, \dots, n-1\}^d$. We enumerate these cubes as Q_i for each $i \in \{1, \dots, n^d\}$. In each cube Q_i we place N_i particles with

$$N_i := \lfloor n^{4d} \rho_i \rfloor, \quad i \in \{1, \dots, n^d\},$$

where $\rho_i := \rho(Q_i)$. These particles are placed at $x_{i,1}, \dots, x_{i,N_i}$ (when $N_i = 0$, no particles are actually placed), anywhere on different points of a square grid obtained by subdividing the sides of Q_i into $\lfloor N_i^{1/d} + 1 \rfloor$ equal smaller intervals, and by taking the nodes whose coordinates are at the centre points of these intervals. Notice that at least one of the ρ_i is larger than or equal to $1/n^d$, so that at least one of the N_i is strictly larger than 0. We write

$$N_p := \sum_{i=1}^{n^d} N_i,$$

the total number of particles placed so far. Let us write $N_e := N - N_p$, the number of particles that we still need to place (with “e” standing for “error”). The numbers N_p and N_e should not be confused with the number N_i of particles placed in the cube Q_i . We observe that

$$N - 4dN^{1-1/(4d)} - N^{1/4} \leq n^{4d} - n^d = \sum_{i=1}^{n^d} (n^{4d} \rho_i - 1) \leq N_p \leq \sum_{i=1}^{n^d} n^{4d} \rho_i = n^{4d} \leq N, \quad (6.2)$$

which yields

$$N_e \leq 4dN^{1-1/(4d)} + N^{1/4}.$$

Of course, if $N_e = 0$ there is nothing left to do. Otherwise, we place the remaining N_e particles at y_1, \dots, y_{N_e} in an auxiliary cube $[3L, 3L + 1/\sqrt{d}]^d$, in different nodes of a uniform square grid with spacing $1/(\sqrt{d} \lfloor N_e^{1/d} + 1 \rfloor)$. The location and size of this auxiliary cube ensure that the distance between any particle in the auxiliary cube and any particle in the main cube $[-L, L]^d$ is greater than $2L$, and that the distance between any two particles in the auxiliary cube is less than 1. The choice of the uniform grid ensures that the Morrey regularity is kept at the discrete level; see Lemma 6.5 below.

We give mass $1/N$ to all the particles thus placed, so that the total mass is 1. We then define the candidate recovery sequence for ρ by gathering all particles placed so far:

$$\mathbf{X}_N^* := (x_{1,1}, \dots, x_{1,N_1}, \dots, x_{n^d,1}, \dots, x_{n^d,N_{n^d}}, y_1, \dots, y_{N_e}) \in \mathbb{R}^{Nd},$$

with the associated empirical measure

$$\mu_{\mathbf{X}_N^*} := \theta_N \mu_N^p + (1 - \theta_N) \mu_N^e,$$

where

$$\mu_N^p := \frac{1}{N_p} \sum_{i=1}^{n^d} \sum_{k=1}^{N_i} \delta_{x_{i,k}}, \quad \mu_N^e := \frac{1}{N_e} \sum_{j=1}^{N_e} \delta_{y_j}, \quad \text{and} \quad \theta_N := \frac{N_p}{N}.$$

Notice that $\theta_N \rightarrow 1$ as $N \rightarrow \infty$, by (6.2). In the following we refer to $x_{1,1}, \dots, x_{n^d,N_{n^d}}$ as the *main* particles, and to y_1, \dots, y_{N_e} as the *auxiliary* particles. In Figure 1 we illustrate the above construction and we summarise the main quantities.

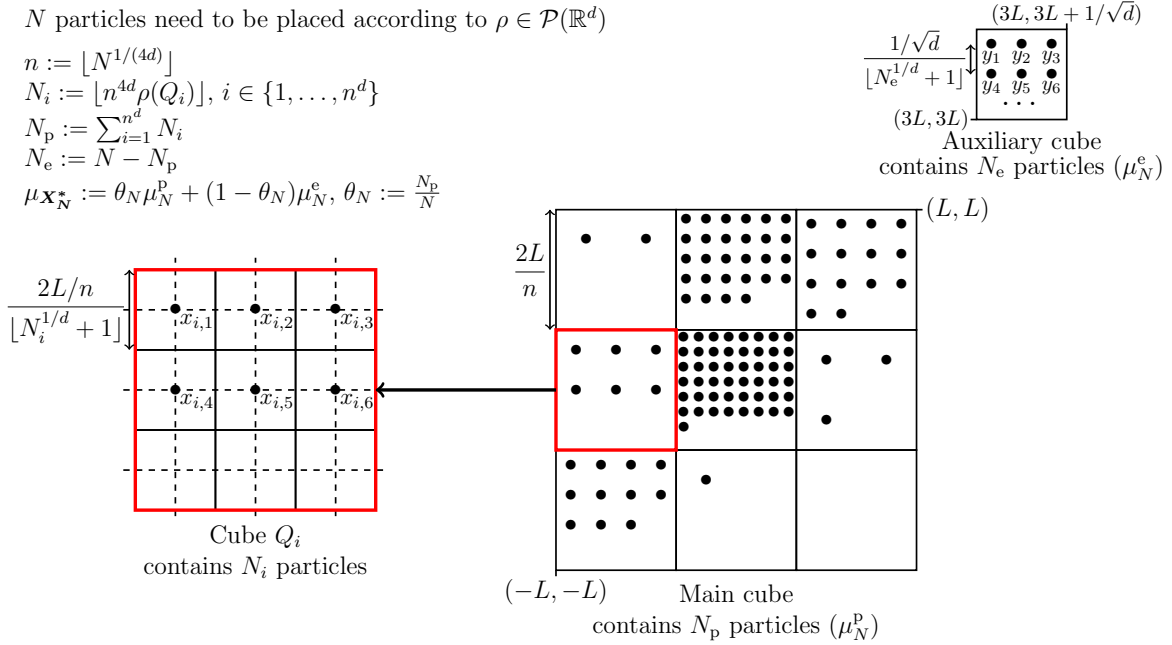


FIGURE 1. Schematic illustration of the construction of the empirical approximation.

6.2.2. Narrow approximation. We show that $(\mathbf{X}_N^*)_{N \geq 2}$ is a good narrow approximation of ρ , which is the first part of the limsup inequality in the compactly supported case; see Definition 6.1. We also prove that if ρ is Morrey regular, so is \mathbf{X}_N^* for all $N \geq 2$.

Lemma 6.5. *Let $\rho \in \mathcal{P}(\mathbb{R}^d)$ be compactly supported. There exists a sequence $(\mathbf{X}_N^*)_{N \geq 2}$ such that*

$$\sigma(\mu_{\mathbf{X}_N^*}, \rho) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

If furthermore $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ for some $p \in [1, \infty)$, then $\mathbf{X}_N^ \in \mathcal{M}_p^N$ for all $N \geq 2$ and $[\mathbf{X}_N^*]_{\mathcal{M}_p^N}$ is uniform in N .*

Let us point out that for a given probability density ρ the problem of finding the best empirical approximation of ρ in some topology for a fixed number of particles is called *quantisation*. Typically ρ is in this context compactly supported and the metric is the Wasserstein distance. In this case the best approximation can be constructed by covering the support of ρ with appropriate balls and using the Voronoi tessellation generated by their centres, and rates of convergence as $N \rightarrow \infty$ can be obtained under suitable regularity of ρ ; see [33, 35]. The empirical approximation constructed in this paper is specific to our problem—we are not concerned with its optimality in approaching ρ but with the fact that it also has to preserve the energy as $N \rightarrow \infty$; see Lemma 6.6.

Proof of Lemma 6.5. Take \mathbf{X}_N^* as in Section 6.2.1. We proceed in two steps.

Step 1: approximation of ρ . Let $\phi \in L^\infty(\mathbb{R}^d) \cap \text{Lip}(\mathbb{R}^d)$ with $\|\phi\|_\infty \leq 1$ and $\|\phi\|_{\text{Lip}} \leq 1$. As already noticed at the beginning of Section 6, the narrow topology is obtained by duality with bounded Lipschitz functions. Hence to prove the result it suffices to prove that $|\int_{\mathbb{R}^d} \phi(x) d\rho(x) - \int_{\mathbb{R}^d} \phi(x) d\mu_{\mathbf{X}_N^*}(x)| \rightarrow 0$ as $N \rightarrow \infty$. First notice that

$$\left| \int_{\mathbb{R}^d} \phi(x) d\rho(x) - \int_{\mathbb{R}^d} \phi(x) d\mu_{\mathbf{X}_N^*}(x) \right| \leq \phi_N + (1 - \theta_N) \left| \int_{\mathbb{R}^d} \phi(x) d\mu_N^e(x) \right| \leq \phi_N + (1 - \theta_N),$$

where $\phi_N := |\int_{\mathbb{R}^d} \phi(x) d\rho(x) - \theta_N \int_{\mathbb{R}^d} \phi(x) d\mu_N^p(x)|$. Since $\theta_N \rightarrow 1$ as $N \rightarrow \infty$ we only need to show that $\phi_N \rightarrow 0$. Using that $n^{4d} - n^d \leq N_p \leq n^{4d}$ and $N_i := \lfloor n^{4d} \rho_i \rfloor$ we get

$$\frac{\rho_i}{N_i + 1} \leq \frac{1}{N_p} \leq \frac{\rho_i}{N_i} + \frac{n^d \rho_i}{N_p N_i} \quad \text{for any } i \in \{1, \dots, n^d\} \quad (6.3)$$

and obtain

$$\left| \frac{1}{N_p} - \frac{\rho_i}{N_i} \right| \leq \max \left(\frac{1}{N_i + 1}, \frac{n^d}{N_p} \right) \frac{\rho_i}{N_i} \leq \frac{\max(1, n^d \rho_i)}{N_p N_i} \leq \frac{n^d}{N_p N_i}.$$

Using this, compute

$$\begin{aligned} \phi_N &= \left| \sum_{i=1}^{n^d} \int_{Q_i} \phi(x) d\rho(x) - \sum_{i=1}^{n^d} \frac{\theta_N}{N_p} \sum_{k=1}^{N_i} \phi(x_{i,k}) \right| \\ &\leq \left| \sum_{i=1}^{n^d} \int_{Q_i} \phi(x) d\rho(x) - \sum_{i=1}^{n^d} \frac{\theta_N \rho_i}{N_i} \sum_{k=1}^{N_i} \phi(x_{i,k}) \right| + \theta_N \sum_{i=1}^{n^d} \frac{n^d}{N_p N_i} \sum_{k=1}^{N_i} |\phi(x_{i,k})| \\ &\leq \left| \sum_{i=1}^{n^d} \frac{\rho_i}{N_i} \sum_{k=1}^{N_i} (\phi(z_i) - \theta_N \phi(x_{i,k})) \right| + \frac{\theta_N n^{2d}}{N_p}, \end{aligned} \quad (6.4)$$

for some $z = (z_1, \dots, z_{n^d}) \in Q_1 \times \dots \times Q_{n^d}$. For the first term in (6.4) we use that the cubes Q_i have a diameter equal to $\sqrt{d}(2L/n)$ to bound it by

$$\sum_{i=1}^{n^d} \frac{\rho_i}{N_i} \sum_{k=1}^{N_i} |\phi(z_i) - \phi(x_{i,k})| + (1 - \theta_N) \sum_{i=1}^{n^d} \frac{\rho_i}{N_i} \sum_{k=1}^{N_i} |\phi(x_{i,k})|$$

$$\leq \sum_{i=1}^{n^d} \frac{\rho_i}{N_i} \sum_{k=1}^{N_i} |z_i - x_{i,k}| + (1 - \theta_N) \leq \frac{2L\sqrt{d}}{n} + (1 - \theta_N).$$

Thus

$$\phi_N \leq \frac{2L\sqrt{d}}{n} + (1 - \theta_N) + \frac{\theta_N n^{2d}}{N_p} \leq \frac{2L\sqrt{d}}{n} + (1 - \theta_N) + \frac{\theta_N n^{2d}}{n^{4d} - n^d},$$

using (6.2). Since $\theta_N \rightarrow 1$ as $N \rightarrow \infty$ we can make the right-hand side above be arbitrarily small as $N \rightarrow \infty$, which shows the result.

Step 2: Morrey regularity. Assume now that ρ is in $\mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$. Any cube Q_i (with side of length $2L/n$) is contained in a ball of radius $\sqrt{d}(2L/n)$, so

$$\rho_i := \rho(Q_i) \leq \left(\frac{2L\sqrt{d}}{n} \right)^{d/q} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)},$$

where $q = p/(p-1)$. Hence the number of points $x_{i,k}$ on each cube Q_i is bounded as

$$N_i = \lfloor n^{4d} \rho_i \rfloor \leq n^{4d} \left(\frac{2L\sqrt{d}}{n} \right)^{d/q} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)}.$$

Therefore the coordinate spacing η between any two main particles $x_{i,k}$ satisfies

$$\begin{aligned} \eta &\geq \frac{2L/n}{\max_{j \in \{1, \dots, n^d\}} N_j^{1/d} + 1} \geq \frac{2L/n}{2 \max_{j \in \{1, \dots, n^d\}} N_j^{1/d}} \geq \frac{L}{n} \left(n^{4d} \left(\frac{2L\sqrt{d}}{n} \right)^{d/q} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} \right)^{-1/d} \\ &= 2^{-1} n^{-4} d^{-1/(2q)} \left(\frac{2L}{n} \right)^{1/p} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)}^{-1/d}. \end{aligned}$$

If $n = 1$, that is, $N < 16^d$, then there is only one main particle placed in $[-L, L]^d$ and we set $\eta = +\infty$ by convention, which trivially satisfies the above inequality. The number of main particles which are placed inside any ball of radius $r > 0$ centred at any $x_{i,k}$ can be estimated by the number of main particles inside a cube of side $2r$ centred at $x_{i,k}$, which is at most $1 + (2r/\eta)^d$. The total mass of μ_N^p inside that ball, not counting the particle at $x_{i,k}$, is therefore bounded by

$$\mu_N^p(B_r(x_{i,k}) \setminus \{x_{i,k}\}) \leq \frac{1}{N} \left(\frac{2r}{\eta} \right)^d \leq \frac{n^{4d} 4^d d^{d/(2q)}}{N} \left(\frac{2L}{n} \right)^{-d/p} r^d \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)}.$$

In particular, when $r \leq 2L/n$, we have

$$\mu_N^p(B_r(x_{i,k}) \setminus \{x_{i,k}\}) \leq (n^{4d}/N) 4^d d^{d/(2q)} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} r^{d/q}.$$

By (6.2) we have $n^{4d}/N \leq n^{4d}/(n^{4d} - n^d) \leq 1/(1 - 8^{-d})$ if $n \geq 2$; if $n = 1$ then $n^{4d}/N \leq 1/2 \leq 1/(1 - 8^{-d})$. Since $2L/n \leq 2L$ and the main and auxiliary cubes are $2L$ apart, for any auxiliary particle y_j we get

$$\mu_N^p(B_r(y_j) \setminus \{y_j\}) = 0.$$

For $r > 2L/n$ we need a different bound. For any ball $B_r(z)$ of radius $r > 0$ and centred at any $z \in \mathbb{R}^d$, call I the set of indices of the cubes Q_i which touch $B_r(z)$:

$$I := \{i \in \{1, \dots, N\} \mid Q_i \cap B_r(z) \neq \emptyset\}.$$

Then

$$\mu_N^p(B_r(z)) \leq \sum_{i \in I} \mu_N^p(Q_i) = \sum_{i \in I} \frac{N_i}{N} \leq \sum_{i \in I} \frac{n^{4d} \rho_i}{N} = \frac{n^{4d}}{N} \rho \left(\bigcup_{i \in I} Q_i \right).$$

The cubes Q_i have diameter $\sqrt{d}(2L/n)$, so $\bigcup_{i \in I} Q_i \subset B_{r+\sqrt{d}(2L/n)}$. Then, using that $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ we obtain

$$\mu_N^p(B_r(z)) \leq \frac{n^{4d}}{N} \left(r + \frac{2L\sqrt{d}}{n} \right)^{d/q} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)}.$$

Hence, for $r > 2L/n$,

$$\mu_N^p(B_r(z)) \leq (n^{4d}/N)(1 + \sqrt{d})^{d/q} \|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} r^{d/q}.$$

Again, $n^{4d}/N \leq 1/(1 - 8^{-d})$.

We now need to find a mass estimate for μ_N^e . If $N_e = 0$ there is nothing to estimate. Otherwise, recall that the auxiliary particles are positioned such that the distance between two closest neighbours is at least $1/(\sqrt{d}[N_e^{1/d} + 1])$. Take $r > 0$ and $y_j \in \mathbb{R}^d$ any auxiliary particle. The number of auxiliary particles inside $B_r(y_j)$ is at most $1 + 2r\sqrt{d}(N_e^{1/d} + 1)$. Thus

$$\mu_N^e(B_r(y_j) \setminus \{y_j\}) \leq N_e^{-1} \left(2r\sqrt{d}(N_e^{1/d} + 1) \right)^d = \left(2r\sqrt{d}(1 + N_e^{-1/d}) \right)^d \leq 4^d d^{d/2} r^d.$$

Since μ_N^e is supported on a set of diameter 1, we also have $\mu_N^e(B_r(y_j) \setminus \{y_j\}) \leq 4^d d^{d/2} r^{d/q}$. For any main particle $x_{i,k}$ we have

$$\mu_N^e(B_r(x_{i,k}) \setminus \{x_{i,k}\}) = 0$$

if $r \leq 2L$, and

$$\mu_N^e(B_r(x_{i,k}) \setminus \{x_{i,k}\}) \leq \mu_N^e(B_r(y_j) \setminus \{y_j\}) \leq 4^d d^{d/2} \leq 4^d d^{d/2} r^{d/q}$$

for any auxiliary particle y_j if $r > 2L \geq 2 > \text{diam}(\text{supp } \mu_N^e) = 1$.

All in all we have shown that there exist $M_p > 0$ and $M_e > 0$ such that, for any z in the set $\{x_{1,1}, \dots, x_{n^d, N_{n^d}}, y_1, \dots, y_{N_e}\}$ and $r > 0$,

$$\mu_{\mathbf{X}_N^*}(B_r(z)) - \frac{1}{N} = \mu_{\mathbf{X}_N^*}(B_r(z) \setminus \{z\}) \leq \theta_N M_p r^{d/q} + (1 - \theta_N) M_e r^{d/q}.$$

Since $\theta_N \leq 1$ this ends the proof. ■

6.2.3. Approximation of the energy. We show that $(\mathbf{X}_N^*)_{N \geq 2}$ gives rise to a good approximation of the continuum energy E , which is the second part of the limsup inequality in the compactly supported case; see Definition 6.1. (Equivalently, we show Lemma 5.3(2) in the compactly supported case—notice that the liminf and limsup inequalities together actually show the convergence of the energy, as stated in Lemma 5.3(2)).

Lemma 6.6. *Suppose that W satisfies Hypotheses 1–3. Take $\rho \in \mathcal{P}(\mathbb{R}^d)$ if W satisfies Hypothesis 3a, or $\rho \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d - \beta)$ if W satisfies Hypothesis 3b. Assume in any case that ρ has compact support. Then*

$$\lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*) = E(\rho).$$

Proof. Notice that $E(\rho) < +\infty$ by boundedness of W or Lemma 3.6. Take \mathbf{X}_N^* as in Section 6.2.1 and Lemma 6.5. Assume first that W satisfies Hypothesis 3a. By Lemma 6.3, E is both upper and lower semicontinuous in the narrow topology (and hence continuous at any ρ with $E(\rho)$ finite); also, Lemma 6.5 tells us that $\sigma(\mu_{\mathbf{X}_N^*}, \rho) \rightarrow 0$ as $N \rightarrow \infty$. Hence the result:

$$\lim_{N \rightarrow \infty} E_N(\mathbf{X}_N^*) = \lim_{N \rightarrow \infty} \left(E(\mu_{\mathbf{X}_N^*}) - \frac{W(0)}{2N} \right) = E(\rho).$$

Assume now that W satisfies Hypothesis 3b. Then, by bilinearity of E_N ,

$$\begin{aligned} & 2 |E(\rho) - E_N(\mathbf{X}_N^*)| \\ & \leq \left| \sum_{i,j=1}^{n^d} \int_{Q_i} \int_{Q_j} W(x-y) d\rho(x) d\rho(y) - \frac{\theta_N^2}{N_p^2} \sum_{\substack{i,j=1 \\ (i,k) \neq (j,\ell)}}^{n^d} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} W(x_{i,k} - x_{j,\ell}) \right| \\ & \quad + \frac{2\theta_N(1-\theta_N)}{N_e N_p} \left| \sum_{i=1}^{n^d} \sum_{k=1}^{N_i} \sum_{j=1}^{N_e} W(x_{i,k} - y_j) \right| + \frac{(1-\theta_N)^2}{N_e^2} \left| \sum_{i=1}^{N_e} \sum_{\substack{j=1 \\ j \neq i}}^{N_e} W(y_i - y_j) \right| \\ & =: S_{0,N} + S_{1,N} + S_{2,N}. \end{aligned} \tag{6.5}$$

Let us first deal with term $S_{0,N}$. We break the i - and j -sums in $S_{0,N}$ into two sets: the set of i, j such that Q_i and Q_j are far apart and its complement. For all $\eta > 0$ we define

$$I_\eta := \{(i, j) \in \{1, \dots, n^d\}^2 \mid \text{dist}(Q_i, Q_j) > \eta\},$$

and we call I_η^c its complement in $\{1, \dots, n^d\}^2$. Pick η small enough and n large enough such that $|x - y| \leq 1$ for all $(x, y) \in Q_i \times Q_j$ and $(i, j) \in I_\eta^c$. We get

$$\begin{aligned} & \left| \sum_{(i,j) \in I_\eta^c} \int_{Q_i} \int_{Q_j} W(x-y) d\rho(x) d\rho(y) - \frac{\theta_N^2}{N_p^2} \sum_{\substack{(i,j) \in I_\eta^c \\ (i,k) \neq (j,\ell)}} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} W(x_{i,k} - x_{j,\ell}) \right| \\ & \leq C_W \sum_{(i,j) \in I_\eta^c} \int_{Q_i} \int_{Q_j} |x-y|^{2-\beta} d\rho(x) d\rho(y) + \frac{\theta_N^2 C_W}{N_p^2} \sum_{\substack{(i,j) \in I_\eta^c \\ (i,k) \neq (j,\ell)}} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} |x_{i,k} - x_{j,\ell}|^{2-\beta} \\ & \leq C_W C_\eta (\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} + \theta_N^2 [\mu_N^p]_{\mathcal{M}_p^N}) \leq C_W C_\eta (\|\rho\|_{\mathcal{M}_p(\mathbb{R}^d)} + \theta_N^2 M_p), \end{aligned} \tag{6.6}$$

where $C_\eta \rightarrow 0$ as $\eta \rightarrow 0$ comes from Lemmas 3.6 and 4.8, using that $\rho \in \mathcal{M}_p(\mathbb{R}^d)$ and $\mu_N^p \in \mathcal{M}_p^N$ with $[\mu_N^p]_{\mathcal{M}_p^N} \leq M_p$ for some $M_p > 0$; see Step 2 in the proof of Lemma 6.5.

For the terms $(i, j) \in I_\eta$ we use (6.3) and $N_p \leq n^{4d}$ to get, for all $i, j \in \{1, \dots, n^d\}$,

$$\begin{aligned} \left| \frac{1}{N_p^2} - \frac{\rho_i \rho_j}{N_i N_j} \right| &\leq \max \left(\frac{N_i + N_j + 1}{(N_i + 1)(N_j + 1)}, \left(2 + \frac{n^d}{N_p} \right) \frac{n^d}{N_p} \right) \frac{\rho_i \rho_j}{N_i N_j} \\ &\leq \frac{\max(N_i + N_j + 1, (2N_p + n^d)n^d \rho_i \rho_j)}{N_p^2 N_i N_j} \leq \frac{3n^{5d}}{N_p^2 N_i N_j} \end{aligned} \quad (6.7)$$

and obtain

$$\begin{aligned} &\left| \sum_{(i,j) \in I_\eta} \int_{Q_i} \int_{Q_j} W(x - y) \, d\rho(x) \, d\rho(y) - \frac{\theta_N^2}{N_p^2} \sum_{(i,j) \in I_\eta} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} W(x_{i,k} - x_{j,\ell}) \right| \\ &\leq \left| \sum_{(i,j) \in I_\eta} \int_{Q_i} \int_{Q_j} W(x - y) \, d\rho(x) \, d\rho(y) \right. \\ &\quad \left. - \theta_N^2 \sum_{(i,j) \in I_\eta} \int_{Q_i} \int_{Q_j} \frac{1}{N_i} \sum_{k=1}^{N_i} \frac{1}{N_j} \sum_{\ell=1}^{N_j} W(x_{i,k} - x_{j,\ell}) \, d\rho(x) \, d\rho(y) \right| \\ &\quad + \theta_N^2 \sum_{(i,j) \in I_\eta} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} \frac{3n^{5d}}{N_p^2 N_i N_j} |W(x_{i,k} - x_{j,\ell})| =: R_{0,N} + R_{1,N}. \end{aligned} \quad (6.8)$$

The remainder term $R_{1,N}$ accounts for the fact that we are substituting $1/N_p^2$ by $\rho_i \rho_j / (N_i N_j)$; see (6.7). We show now that $R_{0,N}$ and $R_{1,N}$ are small. For $R_{0,N}$,

$$\begin{aligned} R_{0,N} &\leq \sum_{(i,j) \in I_\eta} \int_{Q_i} \int_{Q_j} \frac{1}{N_i} \sum_{k=1}^{N_i} \frac{1}{N_j} \sum_{\ell=1}^{N_j} |W(x - y) - \theta_N^2 W(x_{i,k} - x_{j,\ell})| \, d\rho(x) \, d\rho(y) \\ &\leq \sum_{(i,j) \in I_\eta} \int_{Q_i} \int_{Q_j} \frac{1}{N_i} \sum_{k=1}^{N_i} \frac{1}{N_j} \sum_{\ell=1}^{N_j} |W(x - y) - W(x_{i,k} - x_{j,\ell})| \, d\rho(x) \, d\rho(y) \\ &\quad + (1 - \theta_N^2) \sum_{(i,j) \in I_\eta} \frac{\rho_i \rho_j}{N_i N_j} \sum_{k=1}^{N_i} \sum_{\ell=1}^{N_j} |W(x_{i,k} - x_{j,\ell})| =: R'_{0,N} + R''_{0,N}. \end{aligned} \quad (6.9)$$

The terms $x - y$ and $x_{i,k} - x_{j,\ell}$ in $R'_{0,N}$ satisfy $\eta \leq |x - y| \leq 2L\sqrt{d}$ and $\eta \leq |x_{i,k} - x_{j,\ell}| \leq 2L\sqrt{d}$. Thus, since $W \in C^1(\mathbb{R}^d \setminus \{0\})$, there exists $W'_\eta > 0$ with $|W(x - y) - W(x_{i,k} - x_{j,\ell})| \leq W'_\eta(|x - x_{i,k}| + |y - x_{j,\ell}|)$, and, since the diameter of a cube Q_i is $\sqrt{d}(2L/n)$,

$$R'_{0,N} \leq \frac{4W'_\eta L\sqrt{d}}{n}. \quad (6.10)$$

The terms $x_{i,k} - x_{j,\ell}$ in $R''_{0,N}$ also verify $\eta \leq |x_{i,k} - x_{j,\ell}| \leq 2L\sqrt{d}$, and so there exists $W_\eta > 0$ such that $|W(x_{i,k} - x_{j,\ell})| \leq W_\eta$. Hence

$$R''_{0,N} \leq (1 - \theta_N^2) W_\eta. \quad (6.11)$$

Now, for $R_{1,N}$,

$$R_{1,N} \leq \frac{3\theta_N^2 W_\eta n^{7d}}{N_p^2} \leq \frac{3\theta_N^2 W_\eta n^{7d}}{(n^{4d} - n^d)^2}, \quad (6.12)$$

using (6.2). Letting $n \rightarrow \infty$ (that is, $N \rightarrow \infty$) and then $\eta \rightarrow 0$ in this order in (6.6), (6.8), (6.9), (6.10), (6.11) and (6.12) gives that $S_{0,N} \rightarrow 0$ as $N \rightarrow \infty$.

We now deal with terms $S_{1,N}$ and $S_{2,N}$ in (6.5). As the terms $x_{i,k} - y_j$ in $S_{1,N}$ satisfy $2L \leq |x_{i,k} - y_j| \leq 5L\sqrt{d}$ we have that $|W(x_{i,k} - y_j)| \leq W_L$ for some $W_L > 0$ and

$$S_{1,N} \leq 2W_L \theta_N (1 - \theta_N).$$

By Step 2 of the proof of Lemma 6.5 we know that $\mu_N^e \in \mathcal{M}_p^N$ with $[\mu_N^e]_{\mathcal{M}_p^N} \leq M_e$ for some $M_e > 0$. Also, the terms $y_i - y_j$ in $S_{2,N}$ verify $|y_i - y_j| \leq 1$ and, by Hypothesis 3b and Lemma 4.8, we get

$$S_{2,N} \leq (1 - \theta_N)^2 C_W C_d M_e,$$

for some constant $C_d > 0$. Clearly we have $S_{1,N} \rightarrow 0$ and $S_{2,N} \rightarrow 0$ as $N \rightarrow \infty$ since $\theta_N \rightarrow 1$, which concludes the proof. \blacksquare

6.2.4. Extension to noncompactly supported probability measures. We extend Lemmas 6.5 and 6.6 to the case when ρ is not necessarily compactly supported; this finishes the proof of Lemma 5.3 and Theorem 6.2.

We proceed by density. Take $\rho \in \mathcal{P}(\mathbb{R}^d)$ if Hypothesis 3a holds, or $\rho \in \mathcal{M}_p(\mathbb{R}^d) \cap \mathcal{P}(\mathbb{R}^d)$ with $p = d/(d - \beta)$ if Hypothesis 3b holds. Let $(\rho_l)_{l>0}$ be a sequence of compactly supported probability measures such that $\sigma(\rho_l, \rho) \rightarrow 0$ and $E(\rho_l) \rightarrow E(\rho)$ as $l \rightarrow \infty$; for example take ρ_l to be the normalisation of ρ restricted to the ball B_l . By Lemmas 6.5 and 6.6 we can construct a sequence of particles $(\mathbf{X}_{N,l}^*)_{N \geq 2}$ such that $\sigma(\mu_{\mathbf{X}_{N,l}^*}, \rho_l) \rightarrow 0$ and $E_N(\mathbf{X}_{N,l}^*) \rightarrow E(\rho_l)$ as $N \rightarrow \infty$ for any $l > 0$. Therefore, for any subsequence $(\mathbf{Y}_{k,l})_{k \in \mathbb{N}} := (\mathbf{X}_{N_{k,l}}^*)_{k \in \mathbb{N}}$ we have $\sigma(\mu_{\mathbf{Y}_{k,l}}, \rho_l) \rightarrow 0$ and $F_k(\mathbf{Y}_{k,l}) \rightarrow E(\rho_l)$ as $k \rightarrow \infty$, where we write F_k for E_{N_k} . By the triangle inequality,

$$\sigma(\mu_{\mathbf{Y}_{k,l}}, \rho) \leq \sigma(\mu_{\mathbf{Y}_{k,l}}, \rho_l) + \sigma(\rho_l, \rho).$$

Therefore, for any $l > 0$ there exists $k(l) \in \mathbb{N}$ such that $k(l) \rightarrow \infty$ as $l \rightarrow \infty$, and

$$\sigma(\mu_{\mathbf{Y}_{k(l),l}}, \rho) \leq \frac{1}{l} + \sigma(\rho_l, \rho) \rightarrow 0 \quad \text{and} \quad F_{k(l)}(\mathbf{Y}_{k(l),l}) \leq \frac{1}{l} + E(\rho_l) \rightarrow E(\rho)$$

as $l \rightarrow \infty$. This, together with the liminf inequality shown in Section 6.1, proves that the subsequence $(F_{k(l)})_{l>0}$ Γ -converges to E as $l \rightarrow \infty$. For any subsequence $(F_k)_{k \in \mathbb{N}} = (E_{N_k})_{k \in \mathbb{N}}$ we can therefore extract a further subsequence which Γ -converges to E , which in turn shows that $(E_N)_{N \geq 2}$ Γ -converges to E by the Urysohn property of the Γ -convergence; see [8, Proposition 1.44].

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